10803578

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005
NEWS	20	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	21	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	22	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	23	MAR 02	GBFULL: New full-text patent database on STN
NEWS	24	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	25	MAR 03	MEDLINE file segment of TOXCENTER reloaded

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:21:05 ON 12 MAR 2005

=> file registrey
'REGISTREY' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file regis

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:21:18 ON 12 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAR 2005 HIGHEST RN 845457-93-4
DICTIONARY FILE UPDATES: 11 MAR 2005 HIGHEST RN 845457-93-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\31220052.str

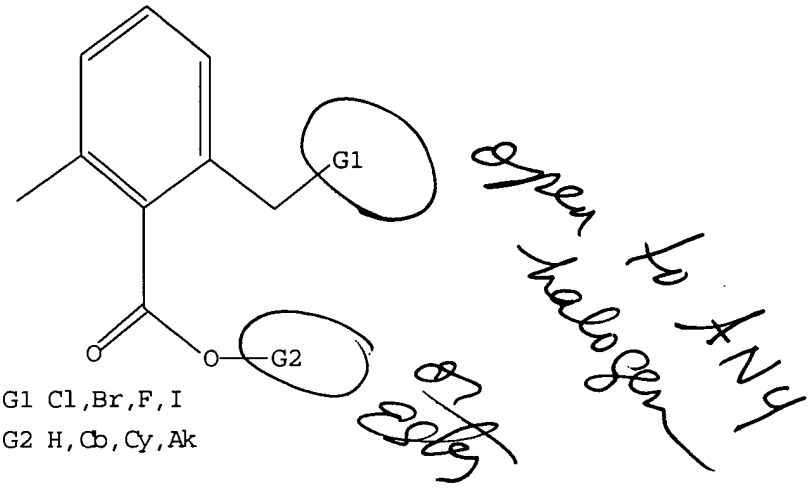
L1 STRUCTURE UPLOADED

=> ad l1
AD IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d l1

10803578

L1 HAS NO ANSWERS
L1 STR



G1 Cl,Br,F,I
G2 H,Cb,Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 13:21:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7840 TO ITERATE

100.0% PROCESSED 7840 ITERATIONS 228 ANSWERS
SEARCH TIME: 00.00.01

L2 228 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 13:22:06 ON 12 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 12 Mar 2005 VOL 142 ISS 12
FILE LAST UPDATED: 11 Mar 2005 (20050311/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

10803578

=> s l2
L3 198 L2

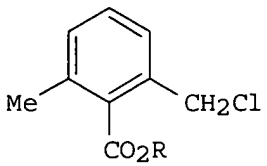
=> d bib abs hitstr 1-198 l3

L3 ANSWER 1 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:802623 CAPLUS
DN 141:314013
TI A preparation of 2-chloromethyl-6-methylbenzoic esters via chlorination of 2,6-dimethylbenzoate esters
IN Maier, Claus-Jurgen; Metzenthin, Tobias; Graeser, Joachim; Bicker, Richard; Manero, Javier
PA Aventis Pharma Deutschland G.m.b.H., Germany
SO U.S. Pat. Appl. Publ., 6 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004192956	A1	20040930	US 2004-803578	20040318
DE 10313228	A1	20041021	DE 2003-10313228	20030325
WO 2004085377	A1	20041007	WO 2004-EP2579	20040312

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI DE 2003-10313228 A 20030325
US 2003-491651P P 20030731
OS CASREACT 141:314013; MARPAT 141:314013
GI



I

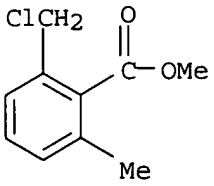
AB The invention relates to a preparation of benzoic ester derivs. of formula I [wherein: R is H, (cyclo)alkyl, (hetero)aryl, or alkyl-aryl, etc.]. The compds. of the formula I are valuable intermediates in the synthesis of PPAR agonists. For instance, Me 2-chloromethyl-6-methylbenzoate was prepared via chlorination of Me 2,6-dimethylbenzoate with a yield of 71% (example 1).

IT **765937-34-6P**, Methyl 2-chloromethyl-6-methylbenzoate
765937-35-7P, Isopropyl 2-chloromethyl-6-methylbenzoate
765937-36-8P, 2-Methoxyethyl 2-chloromethyl-6-methylbenzoate
765937-38-0P, Benzyl 2-chloromethyl-6-methylbenzoate
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of (chloromethyl)(methyl)benzoic esters via chlorination of dimethylbenzoate esters)

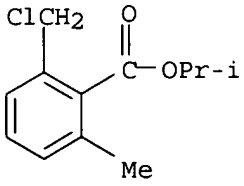
RN 765937-34-6 CAPLUS

CN Benzoic acid, 2-(chloromethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



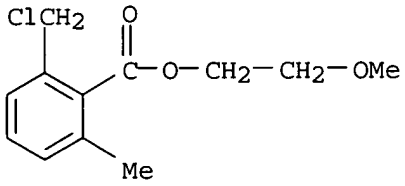
RN 765937-35-7 CAPLUS

CN Benzoic acid, 2-(chloromethyl)-6-methyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



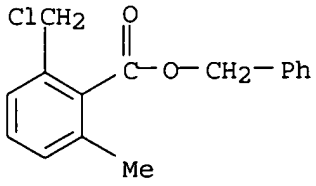
RN 765937-36-8 CAPLUS

CN Benzoic acid, 2-(chloromethyl)-6-methyl-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)



RN 765937-38-0 CAPLUS

CN Benzoic acid, 2-(chloromethyl)-6-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



IT **765937-39-1P**

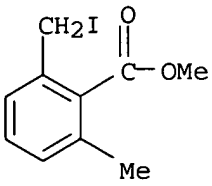
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (chloromethyl)(methyl)benzoic esters via chlorination of dimethylbenzoate esters)

RN 765937-39-1 CAPLUS

CN Benzoic acid, 2-(iodomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX

NAME)



L3 ANSWER 2 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:740279 CAPLUS
DN 141:260285
TI Method for producing the enantiomeric forms of cis-1,3-cyclohexanediol derivatives using an enzymic resolution
IN Holla, Wolfgang; Keil, Stefanie
PA Aventis Pharma Deutschland GmbH, Germany
SO PCT Int. Appl., 91 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004076390	A1	20040910	WO 2004-EP1580	20040219
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	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10308350	A1	20040916	DE 2003-10308350	20030227
	US 2004209931	A1	20041021	US 2004-789053	20040227
PRAI	DE 2003-10308350	A	20030227		
	US 2003-487416P	P	20030715		

OS MARPAT 141:260285
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

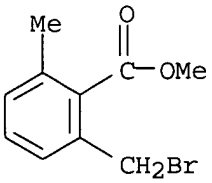
AB The invention relates to a method for producing chiral, non-racemic, disubstituted cis-1,3-cyclohexanediols I [R1 = R'; A = Ph, 5- to 10-membered heteroarom. (containing N, O, S), C8-14-aromatic, C3-8-cycloalkyl; R3 = H, F, Cl, Br, OH, NO2, CF3, OCF3, C1-6-alkyl, C3-8-cycloalkyl, Ph; R4, R5 = H, F, Cl, Br, OH, NO2, CF3, OCF3, OCHF2, OCF2CF3, OCF2CHF2, SCF3, OPh, C1-6-alkyl, O-(C1-6-alkyl), O-(C1-6-alkyl)-O-(C1-3-alkyl); n = 1 - 3; R2 = C1-8-alkyl, optionally, one or more CH2 may be replaced with an O, CO, S, SO, SO2 and substituted with 1 - 3 substituents {F, Cl, Br, CF3, Cn, NO2, NHAc, NHBoc, NHCOCMe3, OH, OCF3, O-(C1-6-alkyl), CO2H, CO2CH2Ph,

CO2-(C1-6-alkyl), tetrazole, indole, (un)substituted thiazolidine-2,4-dione, C6-10-aryl }, or, protecting group (PG) {e.g., CH2OCH2Ph, CH2Ph, CH2C6H4OMe-p, SiMe2CMe3}] using an enzymic resolution of racemates. The preparation of chiral cis-I is characterized by: (a) alkylation of (±)-cis-1,3-cyclohexanediol with R2X1 [X1 = Cl, Br, I, OSO2Me (OMs), OSO2C6H4Me-p (OTs), OSO2CF3 (OTf)] in the presence of a base and a suitable solvent; (b) stereoselective, enzymic resolution of (±)-cis-I (R1 = H) with an acyl donor, R6Cl or (R6)2O [R6 = C(:O)-(C1-16-alkyl), C(:O)-(C2-16-alkenyl), C(:O)-(C3-16-alkynyl), C(:O)-(C3-16-cycloalkyl), optionally one or more CH2 may be replaced with O substituted with 1 - 3 substituents {F, Cl, Br, CF3, CN, NO2, OH, OMe, OEt, Ph, CO2-(C1-4-alkyl), CO2-(C2-4-alkenyl)}], in an organic solvent containing an enzyme; (c) chemical hydrolysis of chiral cis-I (R1 = R6); (d) alkylation of chiral cis-I (R1 = H) with oxazole II (X2 = Cl, Br, I, OTs, OMs, OTf) in the presence of a base and a suitable solvent. Alternatively chiral cis-I is prepared by: (a) alkylation of (±)-cis-1,3-cyclohexanediol with PG-X1 [X1 = Cl, Br, I, OMs, OTs, OTf] in the presence of a base and a suitable solvent; (b) stereoselective, enzymic resolution of (±)-cis-I (R1 = H, R2 = PG) with an acyl donor, R6Cl or (R6)2O, in an organic solvent containing an enzyme; (c) chemical hydrolysis of chiral cis-I (R1 = R6, R2 = PG); (d) alkylation of chiral cis-I (R1 = H; R2 = PG) with oxazole II (X2 = Cl, Br, I, OTs, OMs, OTf) in the presence of a base and a suitable solvent (e) deprotecting chiral cis-I (R2 = PG); (f) alkylation of chiral cis-I (R2 = H) with R2X1 in the presence of a base and a suitable solvent. Thus, cyclohexanediol derivative II was prepared from (±)-cis-1,3-cyclohexanediol via alkylation with Me 2-(bromomethyl)-6-methylbenzoate in NMP containing KOCMe3, enzymic resolution with vinyl acetate in CH2Cl2 containing Novozym 435, alkylation of the resulting chiral (benzyloxy)cyclohexanol III with (iodomethyl)oxazole IV, and saponification with NaOH in EtOH.

IT **56427-77-1P**, 2-(Bromomethyl)-6-methylbenzoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation by, of cis-1,3-cyclohexanediol; prepn of the enantiomeric forms of cis-1,3-cyclohexanediol derivs. using an enzymic resolution)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



Bromide

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:740108 CAPLUS
DN 141:260734
TI Preparation of diarylcycloalkyl oxazole derivatives and their use in the treatment of, e.g., fatty acid metabolism
IN Goerlitzer, Jochen; Glombik, Heiner; Falk, Eugen; Gretzke, Dirk; Keil, Stefanie; Schaefer, Hans-Ludwig; Stapper, Christian; Wendler, Wolfgang
PA Aventis Pharma Deutschland GmbH, Germany
SO PCT Int. Appl., 61 pp.

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CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004075815	A2	20040910	WO 2004-EP1584	20040219
	WO 2004075815	A3	20041229		
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	US 2004204462	A1	20041014	US 2004-789019	20040227
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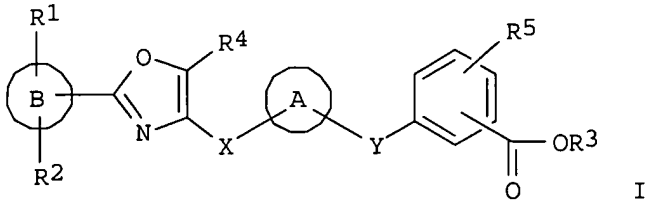
	US 2003-494911P	P	20030813		

OS MARPAT 141:260734
GI



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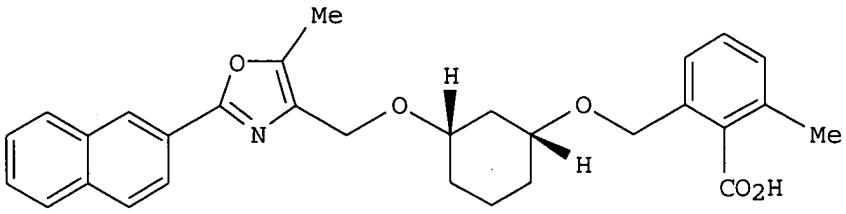


II

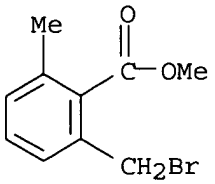
AB Title compds. I [A = cycloalkanediyl, cycloalkenediyl, etc.; B = Ph, heterocyclic, etc.; R1 = SCF3, OCF2-CHF2, phenoxy, etc.; R2 = H, CF3; R3 = H, alkyl; R4 = Ph, H, F, Cl, Br, etc.; R5 = H, F, Cl, Br, OH, etc.; X, Y = alkanediyl, etc.] are prepared For instance, 2-Methyl-6-[(((1R,3S)-3-((5-methyl-2-(naphthalen-2-yl)oxazol-4-yl)methoxy)cyclohexyl)oxy)methyl]benzoic acid (II) is prepared in 7 steps using naphthalene-2-carboxaldehyde, diacetylmonooxime, 1,3-cyclohexanediol and 2-bromomethyl-6-methylbenzoic acid Me ester. II has an EC50 = 0.2 nM for the PPARα receptor. I are useful for treating disorders of the fatty acid metabolism and glucose

utilization in addition to disorders of insulin resistance.

IT **56427-77-1**, 2-Bromomethyl-6-methylbenzoic acid methyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of diarylcycloalkyl oxazole derivs. and their use in treatment of, e.g., fatty acid metabolism)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



Bromide

L3 ANSWER 4 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:738380 CAPLUS

DN 141:260401

TI Preparation of cis-3-(benzyloxy)cyclohexanols as PPAR agonists for the treatment of type II diabetes

IN Stapper, Christian; Glombik, Heiner; Falk, Eugen; Goerlitzer, Jochen; Gretzke, Dirk; Keil, Stefanie; Schaefer, Hans-Ludwig; Wendler, Wolfgang

PA Aventis Pharma Deutschland GmbH, Germany

SO Ger. Offen., 42 pp.
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	WO 2004076402	A1	20040910	WO 2004-EP1583	20040219
	W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004209873	A1	20041021	US 2004-789323	20040227
PRAI	DE 2003-10308352	A	20030227		
	US 2003-487575P	P	20030715		

OS MARPAT 141:260401

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

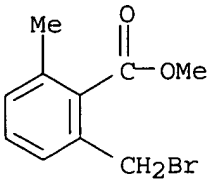
AB Title compds. I [A = (un)substituted cycloalkandiyl (sic) ring, cycloalkendiyl (sic) ring; R = NR1R2, OR1, aryl, etc.; R1, R2 = H, alkyl,

cycloalkyl, etc.; R3 = (un)substituted cycloalkyl, alkyl; R4 = H; R5 = alkyl; X = alkandiyl (sic) with provisos; Y = alkandiyl with provisos] and their pharmaceutically acceptable salts were prepared For example, condensation of phenylisocyanate and amine II, e.g., prepared from 1,3-cyclohexandiol in 5-steps, afforded benzoic acid III. In PPAR-α receptor binding assays, 12-examples of compds. I exhibited EC50 values ranging from 0.07-96 nM, e.g., the EC50 value of benzoic acid III was 1.9 nM. Compds. I are claimed useful for the treatment of type II diabetes.

IT **56427-77-1**, 2-Bromomethyl-6-methylbenzoic acid methyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cis-benzyloxycyclohexanols as PPAR agonists for the treatment of type II diabetes)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:580806 CAPLUS

DN 141:260535

TI Bisacridines with aromatic linking chains. Synthesis, DNA interaction, and antitumor activity

AU Lorente, Antonio; Vazquez, Yolanda; Fernandez, Maria-Jose; Ferrandez, Abel

CS Departamento de Quimica Organica, Universidad de Alcala, Madrid, 28871, Spain

SO Bioorganic & Medicinal Chemistry (2004), 12(16), 4307-4312
CODEN: BMECEP; ISSN: 0968-0896

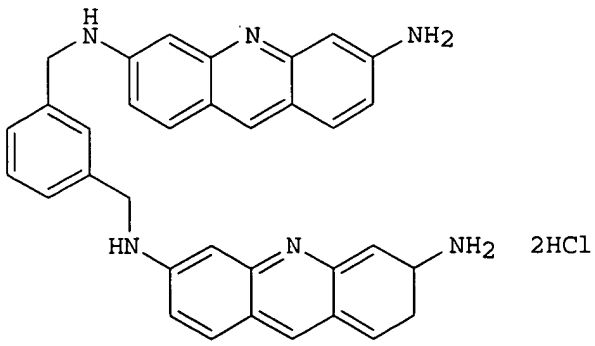
PB Elsevier Ltd.

DT Journal

LA English

OS CASREACT 141:260535

GI



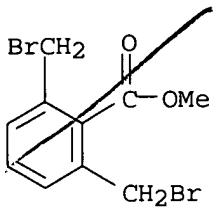
I

AB Synthesis of a series of bisacridine derivs. containing rigid aromatic linking

chains is described. Their DNA interaction and in vitro cytotoxicity against HT-29 human carcinoma cells is reported. An example compound thus prepared and evaluated was N3,N3'-[1,3-phenylenebis(methylene)]bis[1,6-acridinediamine] dihydrochloride (I).

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N3,N3'-[(arenediyl)bis(methylene)]bis[acridinediamine] hydrochlorides using acridinediamine derivs. and bis(bromomethyl)arene derivs. as starting materials)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



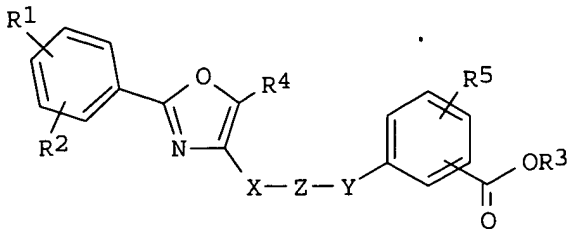
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:513338 CAPLUS
DN 141:71532
TI Method for producing diaryl cycloalkyl derivatives of oxazole and the use thereof as PPAR activators
IN Glombik, Heiner; Falk, Eugen; Frick, Wendelin; Keil, Stefanie; Schafer, Hans-Ludwig; Schwink, Lothar; Wendler, Wolfgang
PA Germany
SO U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 231,432.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

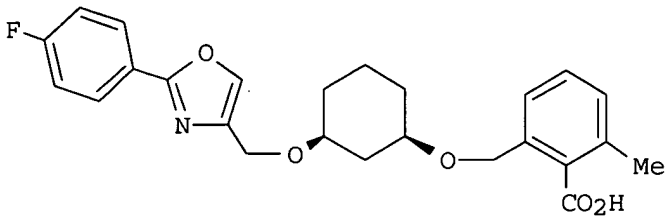
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004122069	A1	20040624	US 2003-631867	20030801
	DE 10142734	A1	20030327	DE 2001-10142734	20010831
	DE 10223273	A1	20031204	DE 2002-10223273	20020524
	US 2003144332	A1	20030731	US 2002-231432	20020830
	US 6624185	B2	20030923		
	ZA 2004001073	A	20040826	ZA 2004-1073	20040210
PRAI	DE 2001-10142734	A	20010831		
	DE 2002-10223273	A	20020524		
	US 2002-231432	A2	20020830		

OS MARPAT 141:71532
GI

10803578



I



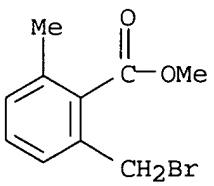
II

AB Title oxazoles I [Z = cycloalkyl; R1, R2, R4, R5 = H, F, Cl, Br, etc.; R3 = H, Me; X, Y = alkyl (chains may contain 1 or more oxygens)] are prepared Thus, (+)-cis-oxazole II was prepared from cyclohexane-1,3-diol via O-alkylation with 4-(Iodomethyl)-2-(4-fluorophenyl)oxazole, separation of cis/trans isomers, HPLC resolution of the cis isomers, and finally alkylation of the (-)-cis isomer with Me 2-(bromomethyl)-6-methylbenzoate. The compds. have lipid and/or triglyceride reducing properties and are suitable e.g. for treating lipid metabolic disorders, type II diabetes and syndrome X. The bioactivity of II was determined [EC50 = 0.3 nM vs. PPARα].

IT **56427-77-1**, Methyl 2-(bromomethyl)-6-methylbenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of cyclohexane-1,3-diol derivative; preparation of oxazole diaryl cycloalkyl derivs. and the use thereof as PPAR activators)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:391288 CAPLUS

DN 140:391286

TI Preparation of water-soluble triazole fungicides

IN Mori, Makoto; Mikoshima, Yoshiko; Koso, Toshiyuki; Shibayama, Takahiro; Uchida, Takuya

PA Sankyo Co., Ltd., Japan

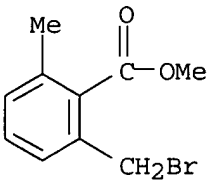
SO Jpn. Kokai Tokkyo Koho, 230 pp.
CODEN: JKXXAF

10803578

DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004137255	A2	20040513	JP 2003-208038	20030820
PRAI	JP 2002-241934	A	20020822		

OS MARPAT 140:391286
AB The title triazole compds. XOCOLOR [wherein X represents such a group that the compound represented by the formula XOH has antifungal activity; L represents (C6-10 aryl)CH2, etc.; further detail on said aryl is given; and R represents P(:O)(OH)2, etc.] are prepared The conversion of one compound of this invention into a fungicidal metabolite by human liver microsomes was demonstrated. A formulation is given.
IT **56427-77-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of water-soluble triazole fungicides)
RN 56427-77-1 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:333680 CAPLUS
DN 140:357669
TI Preparation of peptidyl activity-based probes for catalytically-active enzymes
IN Winn, David; Campbell, David Alan
PA Activx Biosciences, Inc., USA
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004033397	A2	20040422	WO 2003-US32152	20031008
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2002-417664P	P	20021009		

OS MARPAT 140:357669
AB The invention provides compns. and methods for assessing profiles of catalytically-active enzymes (e.g., a hydrolase, most preferably a

cysteine protease) in compns. containing a plurality of proteins. The methods use activity-based probes (ABPs) that have an affinity moiety for directing the binding of the ABP to one or more catalytically-active target enzymes, a reactive group for forming a covalent bond at an active site of the target enzyme(s), and a TAG (e.g., a detectable label, preferably a fluorophore). ABPs TAG-L-CO(NHCHR2CO)nNHCHR1-RG [R1, R2 are H, alkyl optionally containing 1-3 heteroatoms N, O, or S, alkylaryl, -heteroaryl, or -phenyl; RG is a reactive group that reacts to form a covalent bond with a catalytically-active target enzyme; L is optionally present and is an alkyl or heteroalkyl group of 1-20 backbone atoms selected from NR, O, S or CR2, where R is H or alkyl; n is 1-4] or pharmaceutically-acceptable salts or complexes are claimed. One or more ABPs may be combined with a protein-containing sample under conditions for binding and reaction of the ABP(s) with target enzyme(s) that are present in the sample. The resulting products may then be used to assess the active enzyme profile of the sample and can be correlated to the presence, amount, or activity of one or more target enzyme(s) present in the original complex protein mixture An example describes the synthesis of ANP TAMRA-NH(CH2)10CO-L-Asp-CH2OC6HF4-2,3,5,6, where TAMRA is a rhodamine dye.

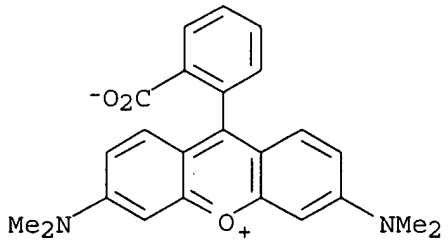
IT **681812-82-8P 681812-85-1P 681812-86-2P 681812-87-3P 681812-89-5P**

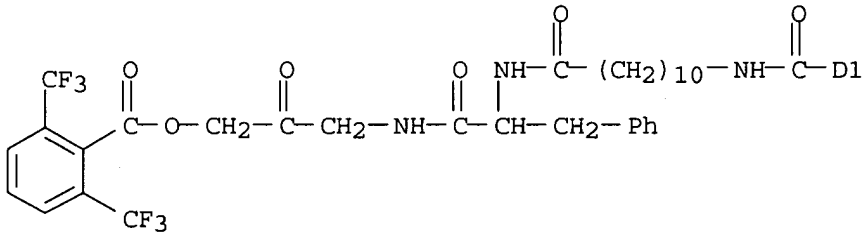
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of peptidyl activity-based probes for catalytically-active enzymes)

RN 681812-82-8 CAPLUS

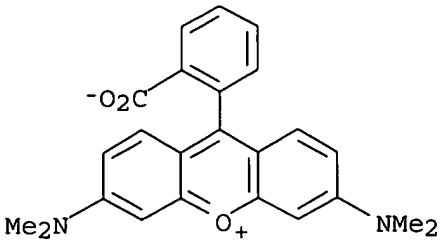
CN Xanthylium, 9-[4(or 5)-[(15S)-22-[2,6-bis(trifluoromethyl)phenyl]-1,13,16,19,22-pentaoxo-15-(phenylmethyl)-21-oxa-2,14,17-triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)

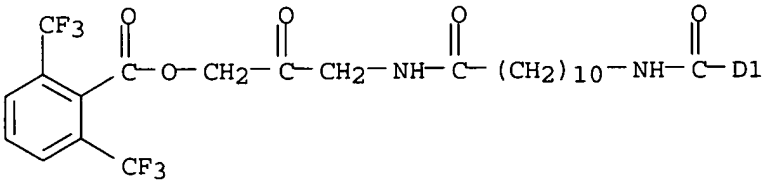




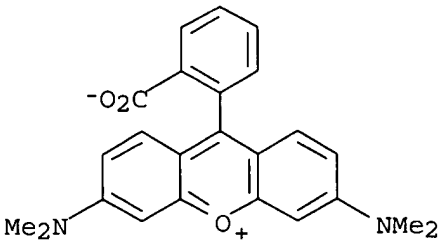
RN 681812-85-1 CAPLUS

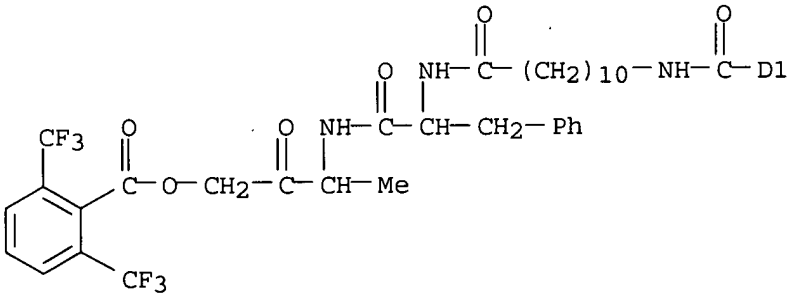
CN Xanthylium, 9-[4(or 5)-[[[11-[[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-2-oxopropyl]amino]-11-oxoundecyl]amino]carbonyl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)



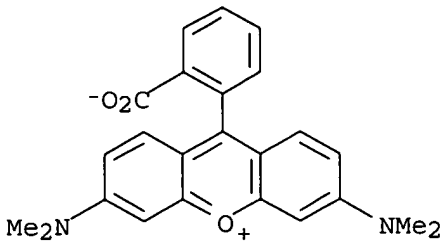


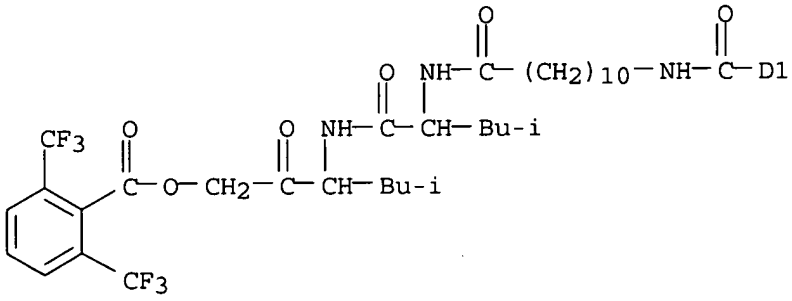
RN 681812-86-2 CAPLUS
CN Xanthylium, 9-[4(or 5)-[(15S,18S)-22-[2,6-bis(trifluoromethyl)phenyl]-18-methyl-1,13,16,19,22-pentaoxo-15-(phenylmethyl)-21-oxa-2,14,17-triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)



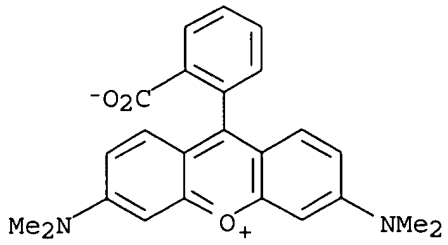


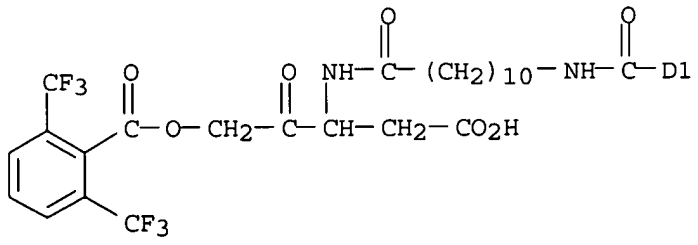
RN 681812-87-3 CAPLUS
CN Xanthylium, 9-[4(or 5)-[(15S,18S)-22-[2,6-bis(trifluoromethyl)phenyl]-15,18-bis(2-methylpropyl)-1,13,16,19,22-pentaoxo-21-oxa-2,14,17-triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





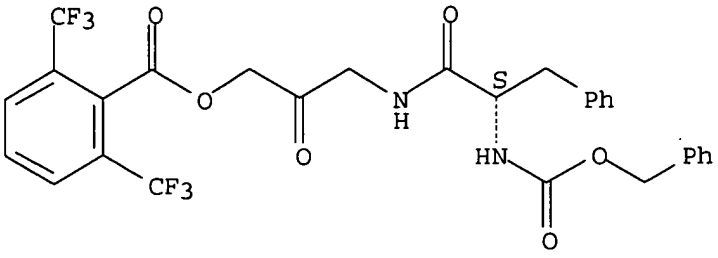
RN 681812-89-5 CAPLUS
CN Xanthylium, 9-[4(or 5)-[[[11-[[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]amino]-11-oxoundecyl]amino]carbonyl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





IT **118253-03-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)
RN 118253-03-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



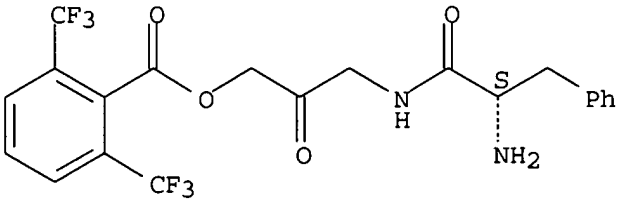
IT **681447-88-1P 681447-89-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)

RN 681447-88-1 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 3-[[(2S)-2-amino-1-oxo-3-phenylpropyl]amino]-2-oxopropyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

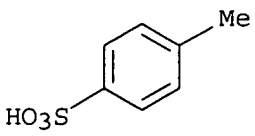
CRN 681447-87-0
CMF C21 H18 F6 N2 O4

Absolute stereochemistry.



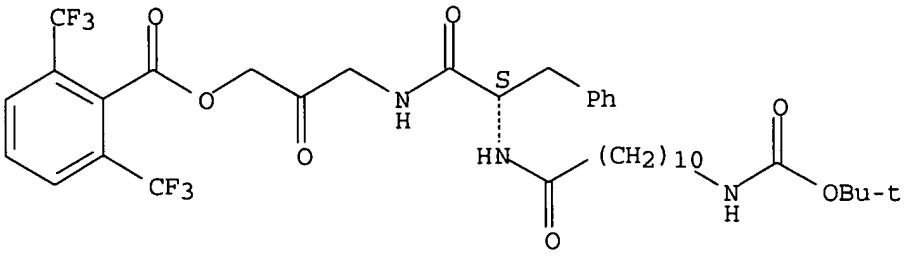
CM 2

CRN 104-15-4
CMF C7 H8 O3 S

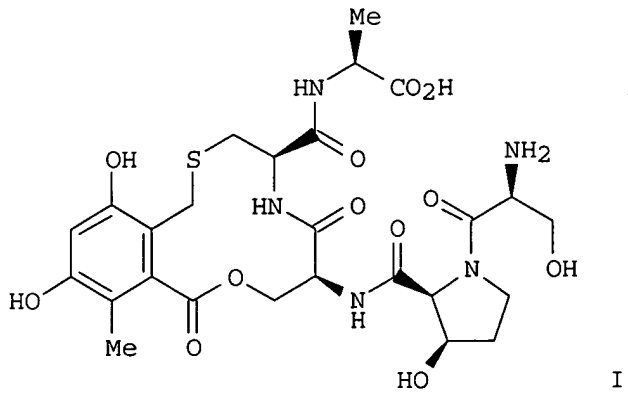


RN 681447-89-2 CAPLUS
CN 2-Oxa-6,9,21-triazadocosan-22-oic acid, 1-[2,6-bis(trifluoromethyl)phenyl]-1,4,7,10-tetraoxo-8-(phenylmethyl)-, 1,1-dimethylethyl ester, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 9 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:90692 CAPLUS
DN 140:304063
TI New Antibacterial Agents Derived from the DNA Gyrase Inhibitor Cyclothialidine
AU Angehrn, Peter; Buchmann, Stefan; Funk, Christoph; Goetschi, Erwin; Gmuender, Hans; Hebeisen, Paul; Kostrewa, Dirk; Link, Helmut; Luebbers, Thomas; Masciadri, Raffaello; Nielsen, Joergen; Reindl, Peter; Ricklin, Fabienne; Schmitt-Hoffmann, Anne; Theil, Frank-Peter
CS Pharmaceutical Division, Preclinical Research, F. Hoffmann-La Roche Ltd., Basel, CH-4070, Switz.
SO Journal of Medicinal Chemistry (2004), 47(6), 1487-1513
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



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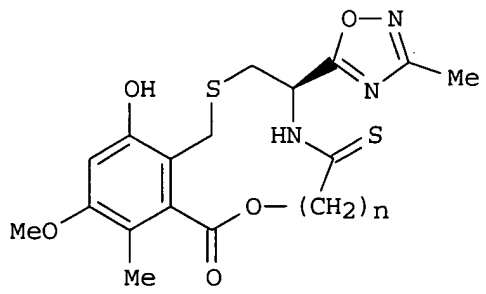


II

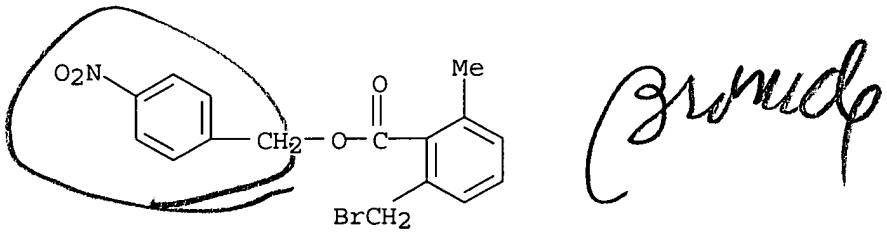
AB Cyclothialidine (I; Ro 09-1437) is a potent DNA gyrase inhibitor that acts

by competitively inhibiting the ATPase activity exerted by the B subunit of DNA gyrase but barely exhibits any growth inhibitory activity against intact bacterial cells, presumably due to insufficient permeation of the cytoplasmic membrane. To explore the antibacterial potential of I, the authors developed a flexible synthetic route allowing for the systematic modification of its structure. From a first set of analogs, structure-activity relationships (SAR) were established for different substitution patterns, and the 14-hydroxylated, bicyclic core of I seemed to be the structural prerequisite for DNA gyrase inhibitory activity. The variation of the lactone ring size, however, revealed that activity can be found among 11- to 16-membered lactones, and even seco-analogs were shown to maintain some enzyme inhibitory properties, thereby reducing the minimal structural requirements to a rather simple, hydroxylated benzyl sulfide. On the basis of these "minimal structures" a modification program afforded a number of inhibitors that showed in vitro activity against Gram-pos. bacteria. The best activities were displayed by 14-membered lactones, and representatives of this subclass exhibit excellent and broad in vitro antibacterial activity against Gram-pos. pathogens, including Staphylococcus aureus, Streptococcus pyogenes, and Enterococcus faecalis, and overcome resistance against clin. used drugs. By improving the pharmacokinetic properties of the most active compds., cyclic lactones II (n = 2, 4), in particular by lowering their lipophilic properties, the authors were able to identify congeners of cyclothialidine that showed efficacy in vivo.

IT **676346-92-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antibacterial activity of structural analogs of cyclothialidine, a DNA-gyrase inhibitor)

RN 676346-92-2 CAPLUS

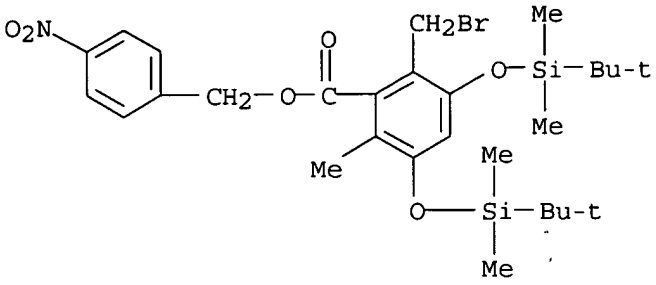
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



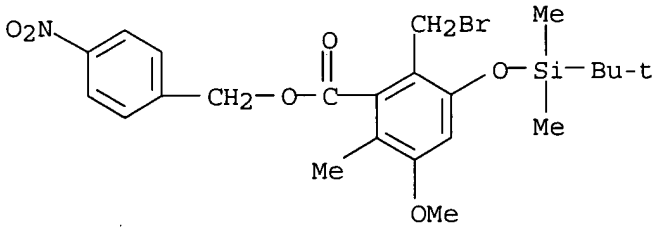
IT **147214-70-8P 147215-10-9P 173152-72-2P**
676347-03-8P 676347-04-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antibacterial activity of structural analogs of cyclothialidine, a DNA-gyrase inhibitor)

RN 147214-70-8 CAPLUS

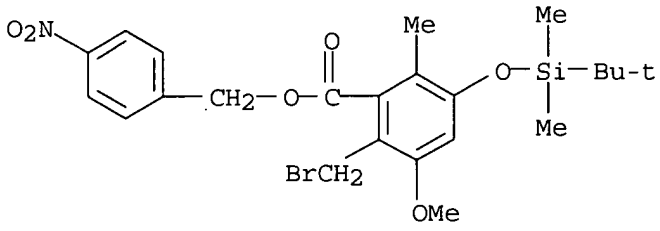
CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



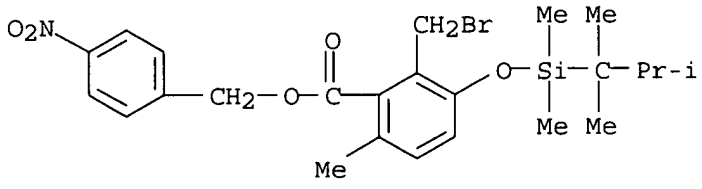
RN 147215-10-9 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-methoxy-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



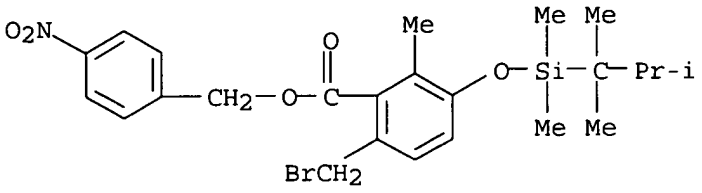
RN 173152-72-2 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methoxy-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



RN 676347-03-8 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3-[[dimethyl(1,1,2-trimethylpropyl)silyl]oxy]-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



RN 676347-04-9 CAPLUS
CN Benzoic acid, 6-(bromomethyl)-3-[[dimethyl(1,1,2-trimethylpropyl)silyl]oxy]-2-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

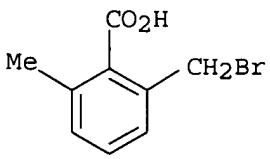


RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:1007924 CAPLUS
DN 140:41909
TI Preparation of 2-bromomethyl-6-methyl-benzoic acid
IN Farina, Paolo; Guidetti, Maurizia
PA Prime Euticals Therapeuticals S.p.A., Italy
SO U.S. Pat. Appl. Publ., 4 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003236431	A1	20031225	US 2003-437996	20030515
	US 6689891	B2	20040210		
	EP 1375467	A1	20040102	EP 2002-13800	20020621
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	EP 2002-13800	A	20020621		

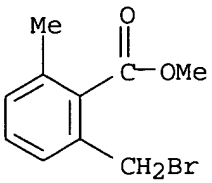
OS CASREACT 140:41909; MARPAT 140:41909
AB The present invention refers to a process for the preparation of 2-bromomethyl-6-methyl-benzoic acid (I) and derivs. thereof by selective bromination of 2,6-dimethylbenzoic acid with sodium bromate and hydrobromic acid in the presence of light. Method of preparation of 7-methyl-3H-isobenzofuran-1-one by cyclization of I in the presence of (iso-Pr)2NEt or in the presence of Na2HCO3, was given. Also, a process for preparation of alkyl esters of I is claimed (examples given).
IT **635316-54-0P**, 2-(Bromomethyl)-6-methylbenzoic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-bromomethyl-6-methyl-benzoic acid)
RN 635316-54-0 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl- (9CI) (CA INDEX NAME)



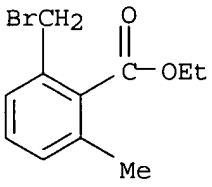
IT **56427-77-1P**, Methyl 2-(bromomethyl)-6-methylbenzoate
635316-53-9P, Ethyl 2-(bromomethyl)-6-methylbenzoate
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-bromomethyl-6-methyl-benzoic acid)
RN 56427-77-1 CAPLUS

10803578

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)

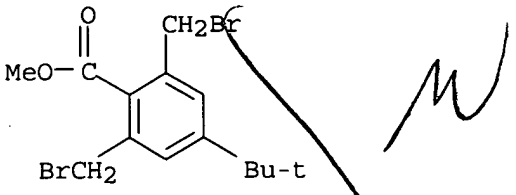


RN 635316-53-9 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 11 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:243018 CAPLUS
DN 139:74577
TI A new cryptophane receptor featuring three endo-carboxylic acid groups: Synthesis, host behavior and structural study
AU Roesky, Christian E. O.; Weber, Edwin; Rambusch, Torsten; Stephan, Holger; Gloe, Karsten; Czugler, Matyas
CS Institut fur Organische Chemie Technische Universitat Bergakademie Freiberg, Freiberg/Sachs, 09596, Germany
SO Chemistry--A European Journal (2003), 9(5), 1104-1112
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Examples of a new type of cryptophane mol. incorporating aromatic groups in the bridges and, for the first time, being also supplied with three endo-positional ionizable carboxylic acid functions have been synthesized and characterized. The cryptophane triester yielded a solvate (channel inclusion compound) with trichloromethane and water, the X-ray crystal structure of which is reported. The complexation of the cryptophane with three endo-carboxylic acid groups with low-mol.-weight alcs. in solution was studied, and the liquid-liquid extraction of different metal ions including alkali (Na+, Cs+), alkaline earth (Mg2+, Ca2+, Sr2+, Ba2+), and the lanthanide metal ions Eu3+ and Yb3+ in an extraction system containing metal nitrate buffer/H2O/1/CHCl3 was examined
IT **119319-00-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting materials in synthesis of cryptophanes)
RN 119319-00-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)

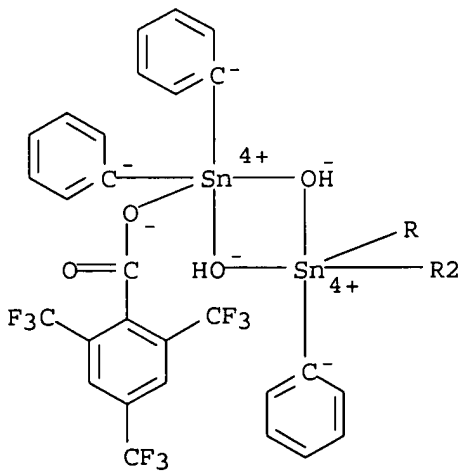
10803578

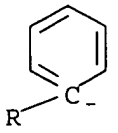


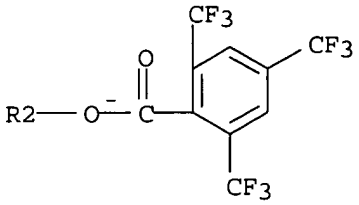
RE.CNT 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:238761 CAPLUS
DN 139:230863
TI First example of a Sn-C bond cleaved product in the reaction of Ph3SnOSnPh3 with carboxylic acids. 3D-Supramolecular network formation in the X-ray crystal structure of [Ph2Sn(OH)OC(O)(Rf)]2, Rf = 2,4,6-(CF3)3C6H2
AU Chandrasekhar, Vadapalli; Nagendran, Selvarajan; Gopal, Kandasamy; Steiner, Alexander; Zacchini, Stefano
CS Department of Chemistry, Indian Institute of Technology, Kanpur, India
SO Chemical Communications (Cambridge, United Kingdom) (2003), (7), 862-863
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 139:230863
AB A 1:2 reaction of Ph3SnOSnPh3 (1) with RfCOOH (2) leads to the formation of [Ph2Sn(OH)OC(O)(Rf)]2 (3) in 94% yield, by means of a facile Sn-C bond cleavage process. The x-ray crystal structure of 3 shows the formation of a three-dimensional supramol. network as a result of three different intermol. secondary interactions.
IT **595584-63-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure, inter mol. bonding, supramol.; reaction of bis(triphenyltin)oxide and tris(trifluoromethyl)benzoic acid in the preparation of diorganostannane dimer)
RN 595584-63-7 CAPLUS
CN Tin, di-μ-hydroxytetraphenylbis[2,4,6-tris(trifluoromethyl)benzoato-κO]di-, stereoisomer (9CI) (CA INDEX NAME)

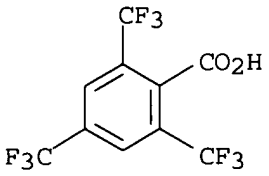
PAGE 1-A







IT **25753-26-8**, 2,4,6-Tris(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of bis(triphenyltin)oxide and tris(trifluoromethyl)benzoic acid in the preparation of diorganostannane dimer)
RN 25753-26-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:202470 CAPLUS
DN 138:238169
TI Method for producing diaryl cycloalkyl derivatives of oxazole and the use thereof as PPAR activators
IN Glombik, Heiner; Falk, Eugen; Frick, Wendelin; Keil, Stefanie; Schaefer, Hans-Ludwing; Schwink, Lothar; Wendler, Wolfgang
PA Aventis Pharma Deutschland GmbH, Germany
SO PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003020269	A1	20030313	WO 2002-EP9221	20020817

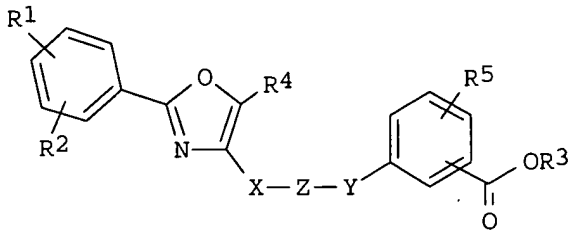
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,

UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

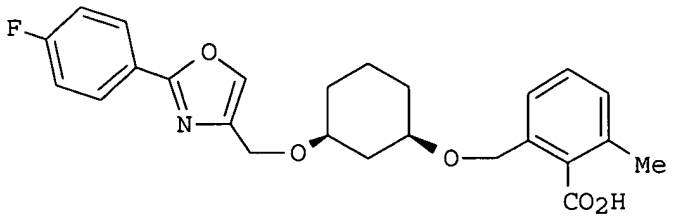
DE	10142734	A1	20030327	DE 2001-10142734	20010831
DE	10223273	A1	20031204	DE 2002-10223273	20020524
EE	200400059	A	20040415	EE 2004-59	20020817
EP	1425014	A1	20040609	EP 2002-797589	20020817
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR	2002012158	A	20040713	BR 2002-12158	20020817
ZA	2004001073	A	20040826	ZA 2004-1073	20040210
PRAI DE	2001-10142734	A	20010831		
DE	2002-10223273	A	20020524		
WO	2002-EP9221	W	20020817		

OS MARPAT 138:238169

GI



I



II

AB The invention relates to diaryl cycloalkyl derivs. and their physiol. compatible salts and physiol. functional derivs. The invention also relates to oxazoles I [Z = C3-8-alkyl, C3-8-alkenyl (rings may contain 1 or more oxygens); R1, R2, R4, R5 = H, F, Cl, Br, OH, NO2, CF3, OCF3, C1-6-alkyl, O-(C1-6-alkyl); R3 = H, C1-6-alkyl; X, Y = C1-6-alkyl (chains may contain 1 or more oxygens)] to their physiol. compatible salts and to a method for producing the same. Thus, (+)-cis-oxazole II was prepared from cyclohexane-1,3-diol via O-alkylation with 4-(Iodomethyl)-2-(4-fluorophenyl)oxazole, separation of cis/trans isomers, HPLC resolution of the cis isomers, and finally alkylation of the (-)-cis isomer with Me 2-(bromomethyl)-6-methylbenzoate. The compds. have lipid and/or triglyceride reducing properties and are suitable e.g. for treating lipid metabolic disorders, type II diabetes and syndrome X. The bioactivity of II was determined [EC50 = 0.3 nM vs. PPARα].

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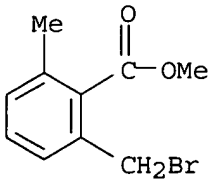
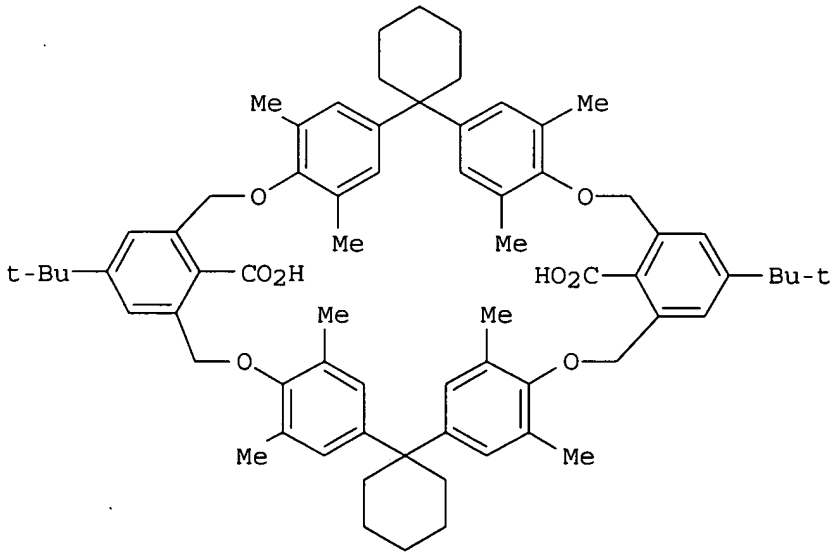
IT **56427-77-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of cyclohexane-1,3-diol derivative; preparation of oxazole diaryl cycloalkyl derivs. and the use thereof as PPAR activators)
RN 56427-77-1 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:44736 CAPLUS
DN 138:321269
TI A New Functional Cyclophane Host. Synthesis, Complex Formation and Crystal Structures of Three Inclusion Compounds
AU Weber, Edwin; Helbig, Cornelia; Seichter, Wilhelm; Czugler, Matyas
CS Institut fuer Organische Chemie der Technischen Universitaet Bergakademie Freiberg, Freiberg/Sachsen, D-09596, Germany
SO Journal of Inclusion Phenomena and Macrocyclic Chemistry (2002), 43(3-4), 239-246
CODEN: JIPCF5; ISSN: 1388-3127
PB Kluwer Academic Publishers
DT Journal
LA English
OS CASREACT 138:321269
GI



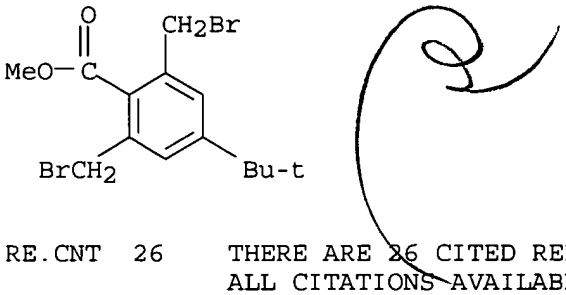
I

AB A new macrocyclic host compound I having an octamethyl substituted

cyclophane structure with two intra-annular carboxylic acid functions has been synthesized via ring closure of bis-benzylic dibromide with diphenol. The properties of crystalline inclusion formation are studied and X-ray crystal structures of three inclusion complexes including acetic acid, propionic acid and acetone as the guest mols. are reported. Inter-host channel formation with complexed guest mols. accommodated into the channels are typical features of the acetic acid and acetone 1:4 (host:guest) stoichiometric complexes being also hydrated species, while the propionic acid 1:2 complex is of the close packing type containing no addnl. water mols. Systems of hydrogen bonds involving the host and guest functional groups are common to all structures. In the case of the acetic acid inclusion compound, a complex supramol. hydrogen-bonded array comprising a bordering tricyclic assembly of eight mol. species exists.

IT **119319-00-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of cyclophane via ring closure of bis-benzylic dibromide with diphenol and crystal structures of their inclusion complexes with solvents)

RN 119319-00-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 15 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:658113 CAPLUS
DN 137:201316
TI Preparation of water-soluble triazole fungicides
IN Mori, Makoto; Kagoshima, Yoshiko; Uchida, Takuya; Konosu, Toshiyuki; Shibayama, Takahiro
PA Sankyo Company, Limited, Japan
SO PCT Int. Appl., 301 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002066465	A1	20020829	WO 2002-JP1500	20020220
W: AU, BR, CA, CN, CO, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PH, PL, RU, SG, SK, US, VN, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2439001	AA	20020829	CA 2002-2439001	20020220
EP 1362856	A1	20031119	EP 2002-701569	20020220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
BR 2002007534	A	20040720	BR 2002-7534	20020220
NZ 527693	A	20041029	NZ 2002-527693	20020220
JP 2002322176	A2	20021108	JP 2002-44541	20020221

10803578

	US 2004198790	A1	20041007	US 2003-647023	20030820
	NO 2003003723	A	20031021	NO 2003-3723	20030821
	ZA 2003006547	A	20040901	ZA 2003-6547	20030821
PRAI	JP 2001-46890	A	20010222		
	WO 2002-JP1500	W	20020220		

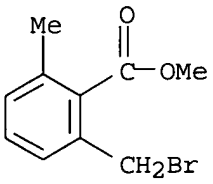
OS MARPAT 137:201316

AB The title triazole compds. XOCOLOR [wherein X represents such a group that the compound represented by the formula XOH has antifungal activity; L represents (C6-10 aryl)CH2, etc.; further detail on said aryl is given; and R represents P(:O)(OH)2, etc.] are prepared The conversion of one compound of this invention into a fungicidal metabolite by human liver microsomes was demonstrated. A formulation is given.

IT **56427-77-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of water-soluble triazole fungicides)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:608624 CAPLUS

DN 137:262833

TI Formation of the Corannulene Core by Nickel-Mediated Intramolecular Coupling of Benzyl and Benzylidene Bromides: A Versatile Synthesis of Dimethyl 1,2-Corannulenedicarboxylate

AU Sygula, Andrzej; Karlen, Steven D.; Sygula, Renata; Rabideau, Peter W.

CS Department of Chemistry and Ames Laboratory, Iowa State University, Ames, IA, 50011, USA

SO Organic Letters (2002), 4(18), 3135-3137
CODEN: ORLEF7; ISSN: 1523-7060

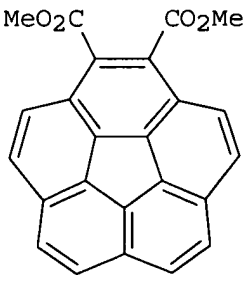
PB American Chemical Society

DT Journal

LA English

OS CASREACT 137:262833

GI



I

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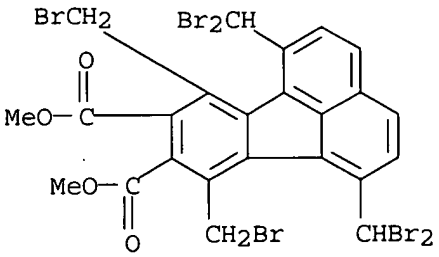
AB A practical synthesis of di-Me 1,2-corannulenedicarboxylate (I) is reported, with the final ring-forming step achieved by the double intramol. nickel powder mediated coupling of benzyl and benzylidene bromide groups with 60% isolated yield.

IT **463327-76-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(practical synthesis of di-Me 1,2-corannulenedicarboxylate involving nickel-mediated intramol. coupling of benzyl and benzylidene bromide groups)

RN 463327-76-6 CAPLUS

CN 8,9-Fluoranthenedicarboxylic acid, 7,10-bis(bromomethyl)-1,6-bis(dibromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:518113 CAPLUS

DN 137:79968

TI Production method of heat-resistant polybenzoxazole-type organic electric insulator films

IN Hatao, Takuya; Hase, Yoko; Enoki, Naoshi

PA Sumitomo Bakelite Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

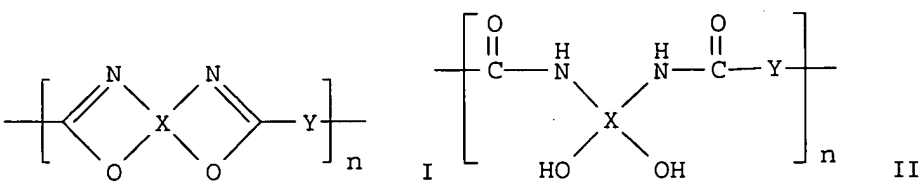
DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002197931	A2	20020712	JP 2000-393498	20001225
PRAI	JP 2000-393498		20001225		

GI



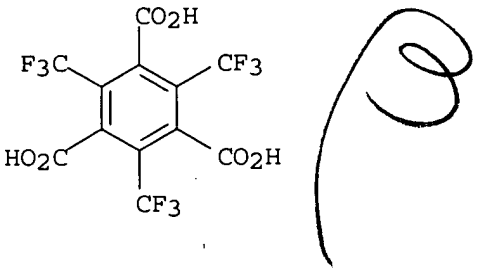
AB Title films comprise a low d. resin layer having main structure unit I prepared by ring closure reaction of a polymeric material II with branch structure after coating on a substrate, where the branched polymeric

material is prepared by reacting (A) a diaminophenol compound (H2N)2X(OH)2 and (B) a d-valent compound having fluoro-containing organic groups, and further reacting with (C) a dicarboxylic acid HOOCYCOOH, wherein d = 3-10 integer; X, Y = benzene ring, biphenyl ring, or (phenyl)2Z; Z = (CH3)2C, (CF3)2C, (CF3)C(phenyl), O, 1,4-phenylene, O-p-C6H4-O, O-p-C6H4-p-C6H4-O, or O-p-C6H4-p-C6H4-p-C6H4-O (optionally H atoms in benzene rings are substituted with Me, Et, Pr, iso-Pr, Bu, iso-Bu, tert-Bu, F, and/or CF3); and n = 2-1000 integer. Thus, 3.70 g 2,2-bis(3-amino-4-hydroxyphenyl)hexafluoropropane and 0.159 g 2,4,6-tri(trifluoromethyl)-1,3,5-benzenetricarboxylic acid chloride (preparation given) were reacted at room temperature for 1 h, 4.12 g 4,4'-hexafluoroisopropylidenediphenyl-1,1'-dicarboxylic acid dichloride (preparation given) was added therein to give an insulator material (Mw = 1.36 + 105 and Mn = 7.0 + 103), 20% varnish of the resulting insulator material was coated on an aluminum-deposited silicone wafer and underwent cyclization reaction at 400° for 3 h to give an insulator film with dielec. constant at 1 MHz 2.38 and 5% weight-loss temperature 515°.

IT **440658-50-4P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate in monomer preparation; preparation of polybenzoxazole heat-resistant elec. insulator films)

RN 440658-50-4 CAPLUS

CN 1,3,5-Benzenetricarboxylic acid, 2,4,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:367288 CAPLUS

DN 136:369714

TI Preparation of novel benzimidazole derivatives for treatment of eosinophilia, bronchial asthma, allergic disease, cancer, and viral infections

IN Mizuguchi, Kiyoshi; Ohzawa, Nobuo; Nakai, Yasuhiro; Matsuura, Kazuyuki; Ohnishi, Shuhei; Kato, Yutaka; Satoh, Tsutomu

PA Mochida Pharmaceutical Co., Ltd., Japan

SO U.S., 47 pp., Cont.-in-part of U.S. Ser. No. 214,274, abandoned.
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6387938	B1	20020514	US 2000-614877	20000712
	WO 9801429	A1	19980115	WO 1997-JP2308	19970703
	W: CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	JP 1996-176711	A	19960705		
	WO 1997-JP2308	A2	19970703		
	US 1998-214274	B2	19981231		

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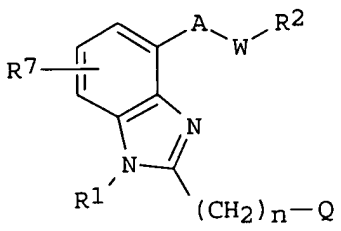
JP 2000-35283 A 20000214
OS MARPAT 136:369714
GI



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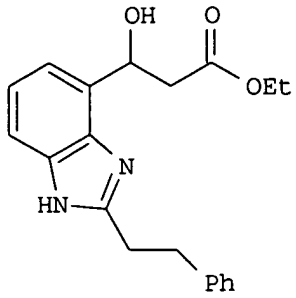
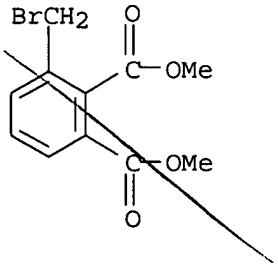


II

AB Title compds. I [wherein R1 = H or alkyl; R2 = cyano, hydroxymethyl, 2-(2-imidazolyl)ethenyl, (un)substituted Ph, CO2R3, or CONR4R5; R3 = H or alkyl; R4 and R5 = independently H, alkyl, CH2CO2R6, CH(CH2Ph)CO2R6; when one of R4 or R5 = CH2CO2R6 or CH(CH2Ph)CO2R6, the other = H; R6 = alkyl; R7 = H, OH, halo, or alkyl; R8 = H or acetyl; R9 = H, acetyl, PhSO2, or (un)substituted benzoyl; A = CO, CH(OR8), CH2O, CH(NHR9)CH2, CH:CH, or CH2CH2; Q = (un)substituted Ph; W = single bond or CH2; n = 0-2; and salts thereof] were prepared as interferon-γ (IFN-γ) enhancers. Thus, CO2(g) was blown into a mixture of 4-acetyl-2-(2-phenylethyl)benzimidazole (preparation given), K2CO3, 18-crown-ether, and DMSO while stirring at room temperature for 6 h to give, after workup, 3-[2-(2-phenylethyl)benzimidazol-4-yl]-3-oxopropanoic acid. Esterification with 25% HCl-EtOH, followed by treatment with NaBH4 in EtOH, afforded II. The latter inhibited the increase of eosinophil counts in mice injected i.p. with pig ascaris extract by 59% at 10 mg/kg/day for 10 days. Oral administration of 10 mg/kg/day, 30 mg/kg/day, and 100 mg/kg/day doses of II for 14 days to tumor-bearing mice enhanced IFN-γ production of spleen cells to 125 pg/mL, 194 pg/mL, and 263 pg/mL, resp., compared to 40 pg/mL for the control. Pharmaceutical formulations, e.g. capsules containing II, were also prepared I are useful for the prevention and/or treatment of eosinophilia, bronchial asthma, and allergic diseases, and may serve as antitumor agents or antiviral agents.

IT **24129-04-2**, 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-, dimethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of benzimidazole derivs. as IFN-γ enhancers for treatment of eosinophilia, bronchial asthma, allergic disease, tumors, and viral infections)

RN 24129-04-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



10803578

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

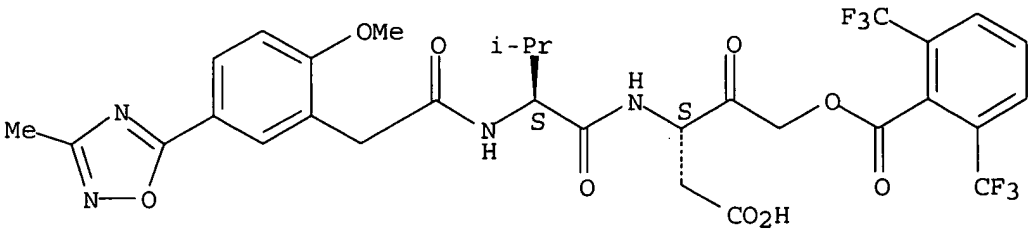
L3 ANSWER 19 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:185062 CAPLUS
DN 136:232548
TI Preparation of γ-keto acid dipeptides as inhibitors of caspase-3
IN Han, Yongxin; Giroux, Andre; Grimm, Erich L.; Aspiotis, Renee; Black, Cameron
PA Merck Frosst Canada & Co., Can.
SO PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002020465	A2	20020314	WO 2001-CA1272	20010906
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2421172	AA	20020314	CA 2001-2421172	20010906
	AU 2001093533	A5	20020322	AU 2001-93533	20010906
	EP 1317414	A2	20030611	EP 2001-973867	20010906
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004521080	T2	20040715	JP 2002-525088	20010906
	US 2002165230	A1	20021107	US 2001-948244	20010907
	US 6525025	B2	20030225		
PRAI	US 2000-231019P	P	20000908		
	WO 2001-CA1272	W	20010906		

OS MARPAT 136:232548
AB γ-Keto acid dipeptides RCR12CONHCR2R3CONHCH(CH2CO2H)COCH2-O-W-Z [W = a bond, CH2, CO or COCH2; Z = H, (un)substituted alkyl, cycloalkyl or a benzofused analog, Ph, naphthyl or a 5- to 10-membered mono- or bicyclic, aromatic or non-aromatic ring, or a benzofused analog, containing 1-3 heteroatoms
selected from O, S and N; R = (un)substituted alkoxyphenyl; R1 = H, halo, OH, alkyl or alkoxy optionally substituted by oxo or 1-3 halo groups; R2 = H, Ph, naphthyl, (un)substituted (cyclo)alkyl; R3 = H or R2R3 represent a 4-7 membered ring optionally containing one heteroatom selected from O, S and N] were prepared as inhibitors of caspase-3. Thus, (3S)-5-[(2-chloro-6-fluorobenzyl)oxy]-3-[[(2S)-2-[[2-(2,5-dimethoxyphenyl)acetyl]amino]-3-methylbutanoyl]amino]-4-oxopentanoic acid was prepared by the solid phase method by loading (S)-FmocNHCH(CH2CO2Bu-t)COCH2Br (Fmoc = fluorenylmethoxycarbonyl) (preparation described) onto a solid support using the technol. described by Webb et al. (1992).
IT **403499-35-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of γ-keto acid dipeptides as inhibitors of caspase-3)
RN 403499-35-4 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (3S)-4-carboxy-3-[[(2S)-2-[[[2-methoxy-5-(3-methyl-1,2,4-oxadiazol-5-yl)phenyl]acetyl]amino]-3-methyl-1-

oxobutyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 20 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:285808 CAPLUS
DN 135:176625
TI Interaction of cigarette smoke and house dust mite allergens on inflammatory mediator release from primary cultures of human bronchial epithelial cells
AU Rusznak, C.; Sapsford, R. J.; Devalia, J. L.; Shah, S. S.; Hewitt, E. L.; Lamont, A. G.; Davies, R. J.; Lozewicz, S.
CS Academic Department of Respiratory Medicine, St Bartholomew's and the Royal London School of Medicine and Dentistry, The London Chest Hospital, London, UK
SO Clinical and Experimental Allergy (2001), 31(2), 226-238
CODEN: CLEAEN; ISSN: 0954-7894
PB Blackwell Science Ltd.
DT Journal
LA English
AB Several studies have shown that exposure to cigarette smoke and/or house dust mite (HDM) can lead to increased airway inflammation in susceptible individuals. The underlying mechanisms, however, are not defined. To investigate the interaction between cigarette smoke and HDM allergen on mediator release from primary cultures of human bronchial epithelial cells. Confluent human bronchial epithelial cell cultures were exposed to cigarette smoke in the absence or presence of HDM allergen and investigated for the release of IL-8, IL-1β, and sICAM-1. Damage to the epithelial cells themselves was assessed by release of 51Cr. On sep. occasions, we investigated the effect of PTL11028, a highly potent and selective Der p1 inhibitor, on HDM allergen-induced release of IL-8, following activation of HDM allergen by incubation with cysteine. The effect of cigarette smoke exposure on the stability of these released mediators in prepared solns. in the absence/presence of reduced glutathione was also studied. Both HDM allergens and short-term (20 min) cigarette smoke exposure led to a significantly increased release of IL-8, IL-1β and sICAM-1 from the epithelial cell cultures. Longer exposure (1-6 h) to cigarette smoke led to a dramatic decrease in the amount of these mediators detected in the culture medium. While incubation of epithelial cultures with HDM allergen did not cause any significant change in the release of 51Cr from pre-loaded cells, cigarette smoke on its own led to a marked, exposure and incubation-time dependent increase in the release of 51Cr. Incubation with HDM allergen led to a significant, dose and time-dependent increase in the release of IL-8, which was further enhanced when the allergen extract was pre-activated with cysteine. This effect was completely abrogated by PTL11028, a novel Der p1 inhibitor. Prepared solns. of various concns. of IL-8, IL-1β and sICAM-1 exposed to cigarette smoke demonstrated a dramatic exposure time-dependent decrease in the detectable amount of these mediators, an effect which was abrogated by GSH. HDM-induced airway inflammation may include Der p-mediated release of

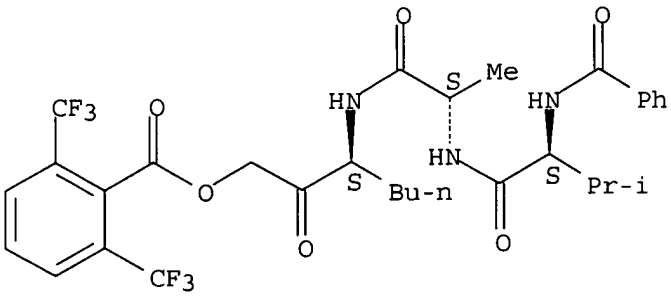
inflammatory mediators from epithelial cells. Addnl., short-term cigarette smoke exposure may induce airway inflammation by release of inflammatory mediators from these cells, an effect which may be potentiated by Der p allergens. Longer term cigarette smoke exposure may cause damage to epithelial cells and changes in the structure of inflammatory mediators.

IT **187991-44-2**, PTL 11028
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(interaction of cigarette smoke and house dust mite allergens on inflammatory mediator release from primary cultures of human bronchial epithelial cells)

RN 187991-44-2 CAPLUS

CN L-Alaninamide, N-benzoyl-L-valyl-N-[(1S)-1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:208279 CAPLUS

DN 134:252327

TI Preparation of 2-(oxalylamino)-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acids as protein tyrosine phosphatase inhibitors

IN Andersen, Henrik Sune; Hansen, Thomas Kruse; Lau, Jesper; Moller, Niels Peter Hundahl; Olsen, Ole Hvilsted; Axe, Frank Urban; Ge, Yu; Holsworth, Daniel Dale; Jones, Todd Kevin; Judge, Luke Milburn; Ripka, Wiliam Charles; Shapira, Barry Zvi; Uyeda, Roy Teruyuki

PA Novo Nordisk A/S, Den.; Ontogen Corp.

SO PCT Int. Appl., 150 pp.
CODEN: PIXXD2

DT Patent

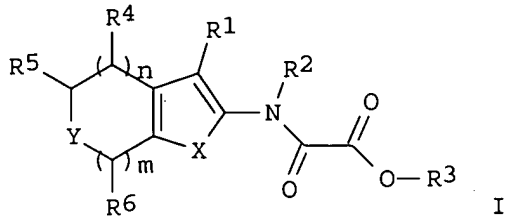
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001019830	A1	20010322	WO 2000-DK502	20000911
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1214324	A1	20020619	EP 2000-958276	20000911

10803578

	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	US 6410556	B1	20020625	US 2000-659547	20000911
	JP 2003509429	T2	20030311	JP 2001-523407	20000911
PRAI	DK 1999-1277	A	19990910		
	DK 2000-1069	A	20000707		
	US 1999-156742P	P	19990930		
	WO 2000-DK502	W	20000911		
OS	MARPAT 134:252327				
GI					



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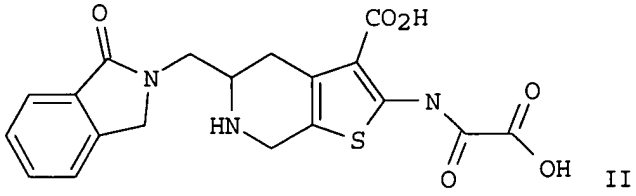


II

AB The title compds. (I) [wherein n = 0-2; m = 1 or 2; X = S or O; Y = O, S, SO, or SO2; R1 = H or CO2R3, tetrazolyl, 3-hydroxyoxazolyl, 3-hydroxyisothiazolyl, 3-hydroxypyrazolyl, 3-hydroxy-1,2,4-oxadiazolyl, 2-thio-1,3,4-oxadiazolyl, 2-hydroxyoxazolyl, 2-hydroxythiazolyl, etc.; R2 = H, alkyl, OH, or NR7R8; R3 = H (ar)alkyl, or alkylcarbonyloxy(ar)alkyl; R4-R6 = independently H, trihalomethyl, (ar)alkyl, (hetero)aryl, OH, oxo, carboxy(alkyl), alkyloxycarbonyl, alkoxy(alkyl), (ar)alkyloxyalkyl, thio, alkylthio, (un)substituted amino, acyl, alkylcarbonylamino(alkyl), etc.; R7 and R8 = independently H, (ar)alkyl, aryl, (ar)alkylcabonyl, arylcarbonyl, or (ar)alkylcarboxy; or R7 and R8 together with the N to which they are attached form an (un)substituted mono-, bi-, or tricyclic ring system containing 0-3 heteroatoms; or R7 and R8 = independently a 5-7 membered amine, imide, or lactam] were prepared as inhibitors of protein tyrosine phosphatases (PTPases), such as PTP1B, CD45, SHP-1, SHP-2, PTPα, LAR, and HePTP. For example, reaction of 2-bromomethyl-3-methoxymethoxybenzoic acid Me ester (preparation given) with 2-amino-5-aminomethyl-6-(4-methoxybenzyl)-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acid tert-Bu ester, amidation using imidazol-1-yloxoacetic acid tert-Bu ester, debenzylation using Pd/C and 10% formic acid in MeOH, and deesterification with 30% TFA afforded II•xTFA (90%). In a study evaluating for biol. activity against a truncated form of PTP1B, II inhibited PTP1B with a Ki of 250 nM. I are useful in the treatment of type I diabetes, type II diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases (no data).

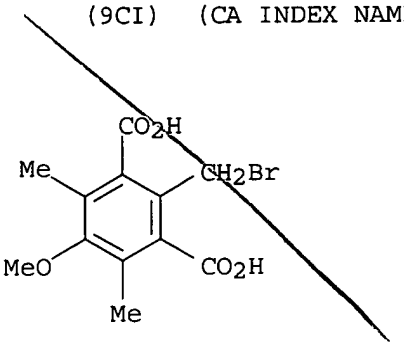
IT **330862-48-1**, 2-Bromomethyl-5-methoxyisophthalic acid dimethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)

10803578

(starting material; preparation of 2-(oxalylamino)-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylic acids as PTP1B inhibitors for treatment of diabetes, impaired glucose tolerance, insulin resistance, obesity, and other diseases)

RN 330862-48-1 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 2-(bromomethyl)-5-methoxy-4,6-dimethyl- (9CI) (CA INDEX NAME)



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:185561 CAPLUS

DN 134:237465

TI Method of inhibiting protein tyrosine phosphatases with an aspartic acid residue at position 48

IN Andersen, Henrik Sune; Hansen, Thomas Kruse; Iverson, Lars Fogh; Lau, Jesper; Moller, Niels Peter Hundahl; Olsen, Ole Hvilsted; Axe, Frank Urban; Ge, Yu; Holsworth, Daniel Dale; Jones, Todd Kevin; Judge, Luke Milburn; Ripka, William Charles; Shapira, Barry Zvi; Uyeda, Roy Teruyuki

PA Novo Nordisk A/S, Den.; Ontogen Corp.

SO PCT Int. Appl., 644 pp.
CODEN: PIXXD2

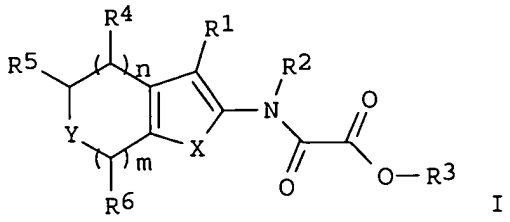
DT Patent

LA English

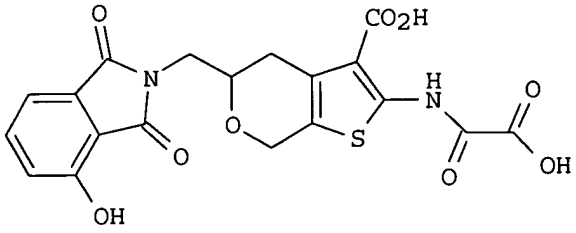
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001017516	A2	20010315	WO 2000-US24761	20000911
	WO 2001017516	A3	20011108		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1214060	A2	20020619	EP 2000-963340	20000911
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	DK 1999-1279	A	19990910		
	US 1999-156641P	P	19990929		
	WO 2000-US24761	W	20000911		

GI



I



II

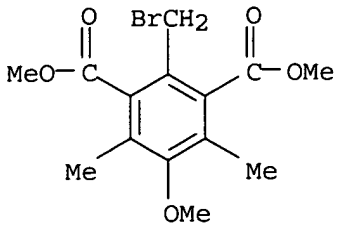
AB The present invention provides a method of inhibiting protein tyrosine phosphatases (PTPases, PTPs), such as PTP1B, TC-PTP, CD45, SHP-1, PTPα, PTPε, PTPβ, PTP D1, PTP D2, PTPH1, and PTP-LAR, by administration of compds. which have structural, phys., and spatial characteristics that allow them to interact with an aspartic acid residue at position 48 of PTP1B and/or TC-PTP. Prepns. for over 100 thieno[2,3-c]pyrans and thieno[2,3-c]pyridines (I) [wherein n = 0-2; m = 0-2; and m = n ≥ 1; X = S, O, NR8; Y = NR8, O, S, SO, SO2; R1 = H, CO2R3, or a 5-membered heterocycle such as tetrazolyl, 3-hydroxyisoxazolyl, 3-hydroxyisothiazolyl, 3-hydroxypyrazolyl, 2-(hydroxy or thio)-1,3,4-oxadiazolyl, 2-oxoimidazolyl, etc.; R2 = H, alkyl, OH, or NR9R10; R3 = H, (ar)alkyl, or alkylcarbonyloxy(ar)alkyl; R4 - R6 = independently H, trihalomethyl, (ar)alkyl, aryl, OH, oxo, CO2H, carboxyalkyl, (ar)alkyloxycarbonyl, alkylaminoalkyl, (ar)alkylcarbonylamino, etc.; R8 - R10 = independently H or (un)substituted (ar)alkyl, aryl, (ar)alkylcarbonyl, arylcarbonyl, or (ar)alkylcarboxy; or R9 and R10 together with the N to which they are attached form an (un)substituted cyclic, bicyclic, or tricyclic ring system containing 0-3 heteroatoms; or R9 and R10 = independently a 5-7 membered cyclic amine, imide, or lactam] and structural-based PTPase inhibition data are included. For example, 5-(4-benzyloxy-1,3-dioxo-1,3-dihydroisoindol-2-ylmethyl)-2-(tert-butoxyoxalylamino)-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid tert-Bu ester was debenzylated using Pd/C and treated with 25% TFA in CH2Cl2 to give II. II showed potency against PTP1B, PTPα D1, PTPε D1, PTPβ, and CD45 D1D2 with Ki values (μM) of 1.9, 93, 11, 1.1, and 130, resp. I are indicated in the management or treatment of a broad range of diseases such as autoimmune diseases, acute and chronic inflammation, osteoporosis, various forms of cancer and malignant diseases, and type I diabetes and type II diabetes (no data). In addition, I are useful in the isolation of PTPases and in elucidation of their biol. function.

IT **330194-70-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; structure-based design and preparation of selective inhibitors of protein tyrosine phosphatases)

RN 330194-70-2 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 2-(bromomethyl)-5-methoxy-4,6-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 23 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:772622 CAPLUS
DN 133:335167
TI Preparation of diaryl carboxylic acids and derivatives as peroxisome proliferator-activated receptor ligands.
IN Jayyosi, Zaid; McGeehan, Gerard M.; Kelley, Michael F.; Labaudiniere, Richard F.; Zhang, Litao; Groneberg, Robert D.; McGarry, Daniel G.; Caulfield, Thomas J.; Minnich, Anne; Bobko, Mark
PA Aventis Pharmaceuticals Products Inc., USA
SO PCT Int. Appl., 167 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

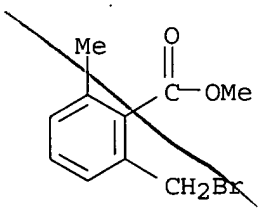
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064888	A1	20001102	WO 2000-US11833	20000428
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2370250	AA	20001102	CA 2000-2370250	20000428
	EP 1177187	A1	20020206	EP 2000-928698	20000428
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000010605	A	20020213	BR 2000-10605	20000428
	EE 200100556	A	20030217	EE 2001-556	20000428
	NZ 515086	A	20031031	NZ 2000-515086	20000428
	US 6635655	B1	20031021	US 2000-662649	20000914
	NO 2001005075	A	20011123	NO 2001-5075	20011018
	ZA 2001008798	A	20030305	ZA 2001-8798	20011024
	HR 2001000795	A1	20030228	HR 2001-795	20011026
PRAI	US 1999-131455P	P	19990428		
	WO 2000-US11833	W	20000428		

OS MARPAT 133:335167
AB Ar1(CR1R2)aA(CR3R4)bAr2(CR5R6)cB(CR7R8)dEZ[Ar1, Ar2 = aryl, fused arylcycloalkenyl, fused arylcycloalkyl, fused arylheterocycloalkenyl, fused arylheterocyclyl, heteroaryl, fused heteroarylcycloalkenyl, fused heteroarylcycloalkyl, fused heteroarylheterocyclyl, etc.; A = O, S, SO, SO2, NR13, CO, NR14CO, CONR15, NR14CONR15, CR14:N, bond, etc.; B = O, S, NR19, bond, CO, NR20CO, CONR20; E = bond, CH2CH2; Z = R21O2C, R21OC, cycloimide, cyano, R21O2SHNCO, R21O2SHN, (R21)2NCO, R21O-substituted 2,4-thiazolidinedionyl, tetrazolyl; a, d = 0-6; b, c = 0-4; R1, R3, R5, R7 = H, halo, alkyl, CO2H, alkoxycarbonyl, aralkyl; R2, R4, R6, R8 = (CH2)qX; q = 0-3; R14, R15, R20 = H, alkyl, aralkyl, CO, alkoxycarbonyl; R14R15 =

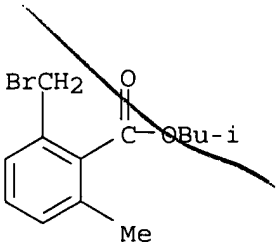
atoms to form a 5-6 membered azaheterocyclyl; R19, R21 = H, aryl, alkyl, cycloalkyl, aralkyl], were prepared as agonists or antagonists of the PPAR receptor (no data). Thus, 3-(quinolin-2-ylmethoxy)propan-1-ol in DMPU/THF at 0° was treated with NaH and then with Me 2-bromomethyl-6-methylbenzoate followed by stirring overnight at room temperature to give Me 2-methyl-6-[3-(quinolin-2-ylmethoxy)propoxymethyl]benzoate.

IT **56427-77-1P 304025-18-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diaryl carboxylic acids and derivs. as PPAR ligands)

RN 56427-77-1 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 304025-18-1 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:772613 CAPLUS
DN 133:335164
TI Tri-aryl acid derivatives as PPAR receptor ligands
IN Jayyosi, Zaid; McGeehan, Gerard M.; Kelley, Michael F.; Labaudiniere, Richard F.; Zhang, Litao; Caulfield, Thomas J.; Minnich, Anne; Bobko, Mark; Morris, Robert; Groneberg, Robert D.; Mcgarry, Daniel G.
PA Aventis Pharmaceuticals Products Inc., USA
SO PCT Int. Appl., 257 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000064876	A1	20001102	WO 2000-US11490	20000428

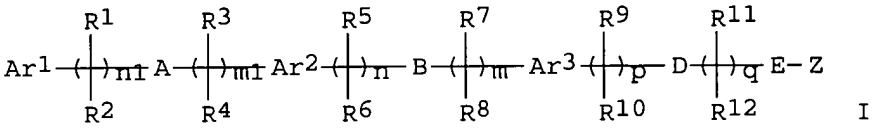
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

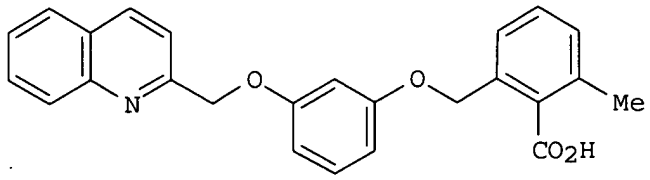
CA 2371308	AA	20001102	CA 2000-2371308	20000428
EP 1177176	A1	20020206	EP 2000-930210	20000428
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010126	A	20020226	BR 2000-10126	20000428
EE 200100558	A	20021216	EE 2001-558	20000428
NZ 515087	A	20031128	NZ 2000-515087	20000428
ZA 2001008800	A	20030210	ZA 2001-8800	20011024
NO 2001005226	A	20011205	NO 2001-5226	20011025
HR 2001000793	A1	20030228	HR 2001-793	20011026
PRAI US 1999-131454P	P	19990428		
WO 2000-US11490	W	20000428		

OS MARPAT 133:335164

GI



I



II

AB This invention is directed to triaryl acid derivs. I and their salts, N-oxides, hydrates, solvates, and pharmaceutical compns. [wherein: Ar1, Ar2, Ar3 = aryl, fused arylcycloalkenyl, fused arylcycloalkyl, fused arylheterocyclenyl, fused arylheterocyclyl, heteroaryl, fused heteroarylcycloalkemyl, fused heteroarylcycloalkyl, fused heteroarylheterocyclenyl, or fused heteroarylheterocyclyl; A = bond, O, S, SO, SO2, CO, (un)substituted NH, NHCO, CONH, NHCONH, CH:N, etc.; B = bond, O, S, SO, SO2, C.tplbond.C, CO, (un)substituted NH, NHCO, or CONH; D = bond, O, S, C.tplbond.C, CO, (un)substituted NH, NHCO, or CONH; E = bond, CH2CH2; Z = (un)substituted CO2H, CHO, cyclo-imide, cyano, sulfonylaminocarbonyl, sulfonylamino, carbamoyl, tetrazolyl, etc.; R1, R3, R5, R7, R9, R11 = H, halo, alkyl, CO2H, alkoxycarbonyl, aralkyl; R2, R4, R6, R8, R10, R12 = (CH2)0-3X (where X = H or various substituents); n1 = 0-4; m1 = 0-4; n = 0-4; m = 0-5; p = 0-4; q = 0-6; with numerous provisos]. The compds. are PPAR receptor ligands, useful as agonists or antagonists thereof (no data). For instance, 2,6-dimethylbenzoic acid underwent a sequence of: (1) Me esterification, (2) benzylic monobromination, (3) etherification with 3-(quinolin-2-ylmethoxy)phenol, and (4) alkaline hydrolysis with NaOH in aqueous EtOH, to give title compound II.

IT **56427-77-1P**

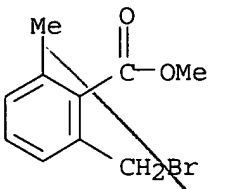
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tri-aryl acid derivs. as PPAR receptor ligands)

RN 56427-77-1 CAPLUS

10803578

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)

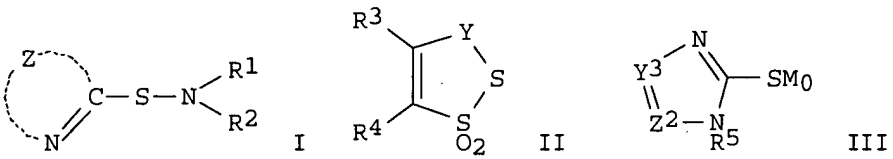


RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:767985 CAPLUS
DN 133:342398
TI Silver halide photographic material and processing thereof
IN Ono, Koji
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 55 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2000305210	A2	20001102	JP 1999-109150	19990416
PRAI JP 1999-109150		19990416		

OS MARPAT 133:342398
GI

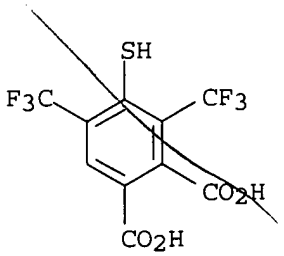


AB The title photog. material possesses a Ag halide emulsion layer containing Ag halide grains which are formed by carrying out grain growth while a solution containing salts is being removed occasionally from the reaction product solution by ultrafiltration in the grain growth process or chemical sensitized with a compound R11R12Au(I)SR13 [R11, R13 = (substituted) aliphatic hydrocarbon, aromatic hydrocarbon, heterocyclic group, R11 and R13 are the same or different; R13 = SO2S, Sk; k = 2-6] and contains a compound I (Z = atoms required to form a 5- or 6-membered heterocycle which may be substituted and condensed with benzene ring; R1, R2 = H, alkyl, aryl, aralkyl, R1 and R2 may link each other to form a N-containing heterocycle) in ≥1 of the constitutive layers. The material may contain the compound I and a compound II [Y = CO, CS, CSe, CH2, (CH2)2; R3, R4 = aliphatic, aromatic or heterocyclic group, atoms required to form a 5- or 6-membered ring or polycyclic system in combination of R3 and R4], A1mY0A2nA3r, or A1mY1A2nA3r-1Z1pY2A1'm1A2'n1A3'r1-1 [A1, A1' = SO3M, CO2M, OM (M = H, metal atom, quaternary ammonium, phosphonium); m, m1, n, n1 = 1-10; A2, A2' =

electron-attracting group; A3, A3' = functional group containing S, Se or Te atom capable of binding to Ag+; r, r1 = 1 or 2; Y0, Y1, Y2 = aliphatic aromatic or heterocyclic group; Z1 = S, Se, Te; p = 1 or 2]. The material is processed with a developing solution containing reductones and 1 selected from I-, sugars, a polyalkylene oxide compound, and a compound III [Y3, Z2 = N, CR6 {R6 = H, (substituted) alkyl, (substituted) aryl}; R5 = alkyl substituted by ≥1 sulfo, CO2H, NH2, OH or its salt or boron residue (when the group has plural substituents, they are the same or different); M0 = H, alkali metal, quaternary ammonium, group capable of becoming H or an alkali metal under alkaline conditions]. The material especially useful in medical use shows high sensitivity, good Ag tone, and low residual color stain in rapid processing using a low replenishment rate and improved storage stability.

IT **237075-93-3**
RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)
(photog. film suited for medical use)

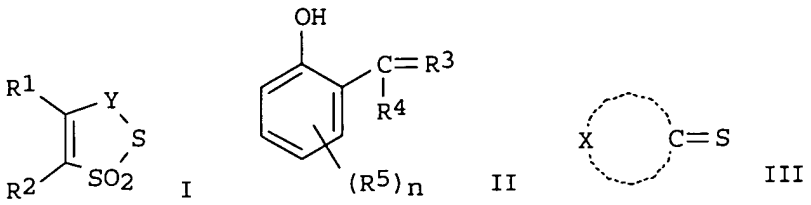
RN 237075-93-3 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-mercapto-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



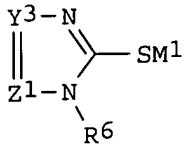
L3 ANSWER 26 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:767984 CAPLUS
DN 133:342397
TI Silver halide photographic material and processing thereof
IN Ono, Koji
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 57 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2000305209	A2	20001102	JP 1999-110797	19990419
PRAI JP 1999-110797		19990419		

OS MARPAT 133:342397
GI



I II III



IV

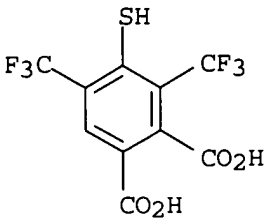
AB The title photog. material, possessing Ag halide emulsion layers and non-photosensitive layers on a support, contains Ag halide grains which are formed by carrying out grain growth while a solution containing salts is being removed occasionally from the reaction product solution by ultrafiltration in the grain growth process or chemical sensitized with a compound R11R12Au(I)SR13 [R11, R13 = (substituted) aliphatic hydrocarbon, aromatic hydrocarbon, heterocyclic group, R11 and R13 are the same or different; R12 = SO2S, Sm; m = 2-6] in ≥1 of the emulsion layers and a compound I [Y = CO, CS, CSe, CH2, (CH2)2; R1, R2 = aliphatic, aromatic or heterocyclic group, atoms required to form a 5- or 6-membered ring or polycyclic system in combination of R1 and R2] in ≥1 of the constitutive layers. The material may contain, in ≥1 of the constitutive layers, the compound I and a compound II (R3 = O, NOH, NH; when R3 = O, R4 = NHOH or NH2, when R3 = NOH or NH, R4 = H, OH, C≤2 alkyl, C≤2 hydroxyalkyl, C≤2 alkoxy; R5 = H, halo, acyl, amino, acylamino, NO2, CN, C≤4 alkyl, alkoxy, OH, CO2H or its salt, sulfo or its salt; n = 0-2), III [X = atoms required to form a heterocycle which has ≥1 group selected from SO3M, CO2M, and OM (M = H, metal atom, quaternary ammonium, phosphonium) directly or indirectly along with the CS group, the heterocycle has no partial structure NHCSNR (R = H, univalent substituent)], A1mYA2nA3r, or A1mY1A2nA3r-1ZpY2A1'm'A2'n'A3'r'-1 [A1, A1' = SO3M, CO2M, OM (M = H, metal atom, quaternary ammonium, phosphonium); m, m', n, n' = 1-10; A2, A2' = electron-attracting group; A3, A3' = functional group containing S, Se or Te atom capable of binding to Ag+; r, r' = 1 or 2; Y, Y1, Y2 = aliphatic aromatic or heterocyclic group; Z = S, Se, Te; p = 1 or 2]. The material is processed with a developing solution containing reductones and 1 selected from I-, sugars, a polyalkylene oxide compound, and a compound IV [Y3, Z1 = N, CR7 {R7 = H, (substituted) alkyl, (substituted) aryl}; R6 = alkyl substituted by ≥1 sulfo, CO2H, amino, OH or its salt or boron residue (when the group has plural substituents, they are the same or different); M1 = H, alkali metal, quaternary ammonium, group capable of becoming H or an alkali metal under alkaline conditions]. The material especially useful in medical use shows high sensitivity, good Ag tone, and low residual color stain in rapid processing using a low replenishment rate and improved storage stability.

IT **237075-93-3**
RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)
(photog. film suited for rapid processing)

RN 237075-93-3 CAPLUS

10803578

CN 1,2-Benzenedicarboxylic acid, 4-mercapto-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 27 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:418038 CAPLUS
DN 133:65901
TI X-ray image formation process
IN Kimura, Sok Man Ho; Amitani, Koji
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 62 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2000171947	A2	20000623	JP 1998-344288	19981203
PRAI	JP 1998-344288		19981203		

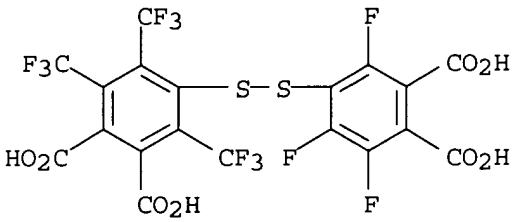
OS MARPAT 133:65901
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB In the process, Ag halide photog. materials contain R21SmR22 (R21, R22 = aliphatic, aromatic, heterocyclic; R21 and R22 may be bonded with S to form ring; m = 2-6 integer). The Ag halide particles are treated with S, Se, and/or Te sensitizers or compds. shown as [A1(W1)r1][[L1(W2)r2]m1[Z1(W3)r3]]n1 (A1 = substituent containing mesoionic compds.; L1 = divalent linkage; Z1 = aromatic group containing unstable chalcogen site; ≥1 of W1-W3 are substituents with CO2H, SO3H, SO2H, phosphoric acid group, phosphorous acid group, boric acid group; m1 = 0, 1; n1 = 1-3; r1-r3 = 0-2; r1 ≠ r2 ≠ r3 ≠ 0). The photog. materials are spectrally sensitized in the presence of Ag halide adsorbents. The spectral sensitizers are shown as I-IV (Z11, Z12, Z21, Z22, Z31, Z41, Z42 = atom. group for forming 5- or 6-membered single ring or N-containing heterocyclic ring; Q31, Q32, Q41 = O, S, Se, NR; R = alkyl, aryl, heterocyclic; R11, R12, R21, R22, R31, R41, R43 = aliph; R32, R33, R42 = aliphatic, aryl, heterocyclic; R13-R17, R23-R29, R34-R39, R44-R49 = H, alkyl, alkoxy, aryloxy, aryl, NW1W2, SR, heterocyclic; R = alkyl, aryl, heterocyclic; W1, W2 = alkyl, aryl; W1, W2 may be bonded and form 5- or 6-membered N-containing heterocyclic ring; R11 and R13, R14 and R16, R17 and R12, R21 and R23, R24 and R26, R25 and R27, R26 and R28, R22 and R29, R31 and R34, R35 and R37, R36 and R38, R41 and R44, R45 and R47, R49 and R43 may be bonded together and form 5- or 6-membered ring or their condensed ring; X11, X21, X41 = ion to compensate the charge in the mol.; m11, m21, m41 = number of ion to compensate the charge in the mol.; n21, n22, n31, n41, n42, l31-l33, l41-l43 = 0, 1; when

142 = 0, 141 = 142 = 0). The pH of the Ag halide emulsions when adding spectral sensitizers is 3-5, then chemical sensitizers are added in the system at pH higher in 0.5-5 than the above pH. The process offer fine images.

IT **276869-74-0**
RL: MOA (Modifier or additive use); USES (Uses)
(antifogging agent; in x-ray image formation process)
RN 276869-74-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-[(3,4-dicarboxy-2,5,6-trifluorophenyl)dithio]-3,5,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 28 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:166114 CAPLUS
DN 132:229558
TI Heat development photographic material using chemically sensitized silver halide and image formation
IN Kimura, Sok Man Ho
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 40 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

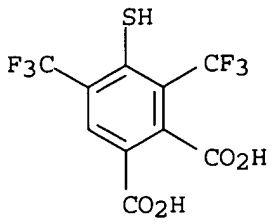
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000075438	A2	20000314	JP 1998-243399	19980828
PRAI JP 1998-243399		19980828		

AB The title photog. material possesses, on a support, a photosensitive layer containing organic Ag salts, binders, and photosensitive Ag halides which have been subjected to ≥1 chemical sensitization selected from S-, Se-, and Te-sensitization in the presence of ≥1 compound R21SmR22 (R21, R22 = aliphatic, aromatic or heterocyclic group, R21 and R22 may link each other to form a ring along with Sm; m = 2-6). To the material may be added a compound A1qYA2nA3r [A1 = SO3M, CO2M, OM (M = H, metal atom, quaternary ammonium, phosphonium); A2 = electron-attracting group; A3 = S-, Se- or Te-containing functional group capable of binding to Ag+; Y = aliphatic, aromatic or heterocyclic group; q, n = 1-10; r = 1 or 2] after ≥1 chemical sensitization selected from S-, Se- and Te-sensitization. An imaging method is also claimed, in which the material is exposed by using lasers. The material shows high sensitivity and storage stability and provides high contrast and low fog images with improved storage stability.

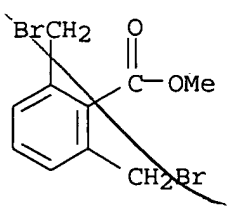
IT **237075-93-3**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(heat-developable photog. film using silver halide chemical sensitized in presence of sulfur compound)
RN 237075-93-3 CAPLUS

10803578

CN 1,2-Benzenedicarboxylic acid, 4-mercapto-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 29 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:119093 CAPLUS
DN 132:216106
TI The first dicopper(II) complex of a new bis(1,5,9-triazacyclododecane) ligand: synthesis, crystal structure and magnetic coupling of the complex
AU Bu, Xian-He; Lu, Shou-Liang; Zhang, Ruo-Hua; Liao, Dai-Zheng; Aoki, Shin; Clifford, Thomas; Kimura, Eiichi
CS Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SO Inorganica Chimica Acta (2000), 298(1), 50-56
CODEN: ICHAA3; ISSN: 0020-1693
PB Elsevier Science S.A.
DT Journal
LA English
AB A new binucleating macrocyclic polyamine ligand based on 1,5,9-triazacyclododecane ([12]aneN3), 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoic acid (HL), was synthesized from a selectively Boc protected [12]aneN3 precursor and 2,6-bis(bromomethyl) benzoate. L can form a stable binuclear complex with Cu(II) in aqueous solution, [Cu2L(N3)2]ClO4, which was characterized by x-ray crystallog. (monoclinic, space group Cc, R = 0.069). The intramol. binuclear Cu(II) centers are bridged by a μ-carboxyl group on L and separated by 5.947 Å. Both of the Cu(II) centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one oxygen of the carboxyl group, as well as one azide anion, and each Cu(II) center is in a distorted state intermediate between a square-pyramid and trigonal-bipyramid environment. This is the 1st binuclear Cu(II) complex formed with a bis([12]aneN3) ligand. Variable temperature magnetic susceptibility studies indicate that there exists intramol. antiferromagnetic coupling (-2J = 71.4 cm-1) between the two unpaired electrons of the two Cu(II) ions in the complex.
IT **56263-51-5**, Methyl 2,6-Bis(bromomethyl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of copper(II) bis(triazacyclododecanylmethyl)benzoato azido dinuclear complex)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



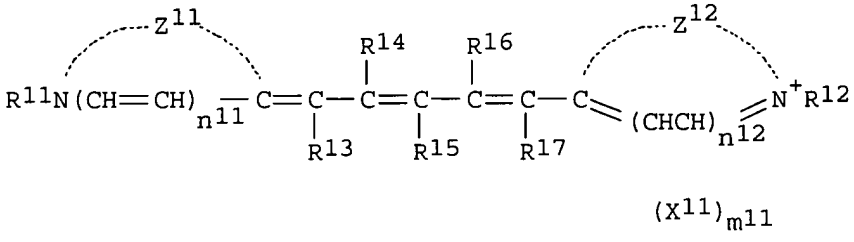
10803578

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 30 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:814651 CAPLUS.
DN 132:57182
TI Heat-developable photographic material containing photosensitizing dye and sulfur compound and image formation using the same
IN Ho, Sokuman; Kakawa, Nobuaki
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 67 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 11352628	A2	19991224	JP 1999-103662	19990412
	US 6214533	B1	20010410	US 1999-286056	19990405
	EP 949537	A2	19991013	EP 1999-302808	19990412
	EP 949537	A3	20000301		
	EP 949537	B1	20020731		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	JP 1998-98910	A	19980410		

GI

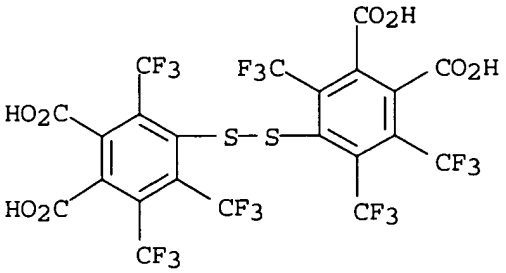


I

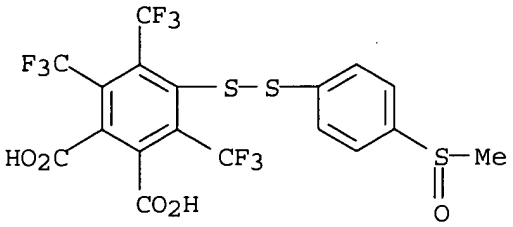
AB The heat-developable photog. material having ≥1 emulsion layer containing an organic Ag salt, a binder, and a photosensitive Ag halide on a support contains (A) ≥1 photosensitive dye such as I (Z11,12 = nonmetal atoms forming N-containing 5- or 6-membered heterocyclyl; R11-17 = aliphatic group; X11 = ion; m11 = number of ions needed to neutralize the dye; n 11,12 = 0, 1) and (B) ≥1 sulfur compound R21(Sm)R22 (R21,22 = aliphatic, aromatic, heterocyclyl; m = 2-6) . The process involving an exposure using an IR laser and a development at 80-200° is also claimed. The heat-developable photog. material shows good storage stability, high sensitivity to IR laser, and gives high contrast images without fog.

IT **252988-67-3 252988-68-4**
RL: DEV (Device component use); MOA (Modifier or additive use); USES (Uses)
(heat-developable photog. material containing photosensitizing dye and sulfur compound)

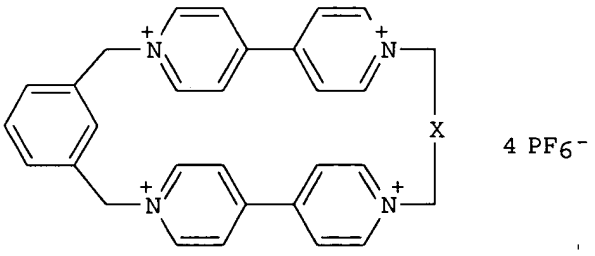
RN 252988-67-3 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4,4'-dithiobis[3,5,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 252988-68-4 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-[[4-(methylsulfinyl)phenyl]dithio]-3,5,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 31 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:559574 CAPLUS
DN 131:271823
TI Synthesis and structures of novel pyridine-bridged phanes of 4,4'-bipyridine
AU Scheytza, Holger; Rademacher, Otto; Reissig, Hans-Ulrich
CS Institut Organische Chemie, Technische Univ. Dresden, Dresden, D-01062, Germany
SO European Journal of Organic Chemistry (1999), (9), 2373-2381
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 131:271823
GI



I

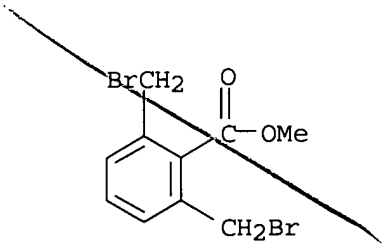
AB Syntheses of novel phanes derived from 4,4'-bipyridine incorporating new spacer elements are described together with their structural and spectroscopic properties. Starting from a pyridine-bridged bis(4,4'-bipyridinium) dication and various bis(bromomethyl) arenes,

macrocycles I (X = 1,2-C6H4, 1,3-C6H4, 1,4-C6H4, 2,6-pyridinediyl, 1,3-C6H4-2-OMe) were prepared in a simple heterogeneous liquid-liquid reaction in satisfactory yields. In complementary expts. starting from bis(4,4'-bipyridinium) compds. with substituted xylenes as spacers, ring closure was performed with 2,6-bis(bromomethyl)pyridine to furnish the corresponding macrocyclic compds. in low yield. Temperature-dependent NMR studies of the macrocycles were performed to investigate their conformational behavior. The x-ray crystal structures for I (X = 1,2-C6H4, 1,3-C6H4, 2,6-pyridinediyl) illustrate the preferred anti-conformation of the macrocycles in the solid state. Consecutive reactions at the pyridine bridge were not successful. However, anisolo-phane I (X = 1,3-C6H4-2-OMe) was converted into the corresponding 4-nitroanisolo-phane by nitration in excellent yield.

IT **56263-51-5**, Methyl 2,6-bis(bromomethyl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridine-bridged phanes of bipyridine)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

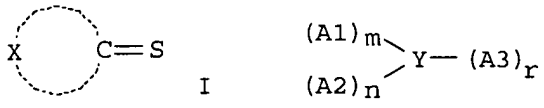


RE.CNT 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 32 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:472037 CAPLUS
DN 131:163301
TI Heat-developable photographic material with improved developed image stability
IN Ho, Sokuman
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 29 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

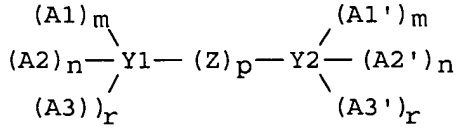
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 11202444	A2	19990730	JP 1998-6559	19980116
PRAI JP 1998-6559		19980116		

OS MARPAT 131:163301
GI

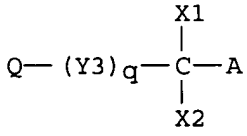


I

II



III



IV

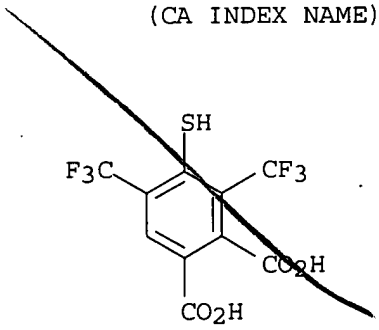
10803578

AB The title photog. material contains I (X = atoms forming heterocycle containing -SO3M, -XOOM and/or -OM; M = H, metal, quaternary ammonium, phosphonium), II or III (A1, A1' = -SO3M, -COOM, -OM; M = H, metal, quaternary ammonium, phosphonium; m = 1-10; A2, A2' = electron withdrawing group; n = 1-10; A3, A3' = function group containing S, Se, or Te; r = 0, 1; Y, Y1, Y2 = aliphatic, aromatic, heterocyclyl; Z = S, Se, Te; p = 1, 2). The material may contain addnl. IV (Q = aryl, heterocyclyl; X1, X2 = halo; Y3 = CO, SO, SO2; A = H, halo, electron withdrawing group; q = 2-6). The material shows reduced fog, improved color tone, storage stability, and developed image stability.

IT **237075-93-3**
RL: DEV (Device component use); USES (Uses)
(in heat-developable photog. material with improved developed image stability)

RN 237075-93-3 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-mercapto-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 33 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:411134 CAPLUS

DN 131:138432

TI Synthesis, crystal structure and magnetic properties of a new dicopper(II) complex with a bis(macrocyclic) ligand

AU Bu, Xian-He; Chen, Wei; Zhang, Ruo-Hua; Chen, Rong-Ti

CS Dep. Chem., Nankai Univ., Tianjin, 300071, Taiwan

SO Huaxue Xuebao (1999), 57(6), 627-634
CODEN: HHHPA4; ISSN: 0567-7351

PB Kexue Chubanshe

DT Journal

LA Chinese

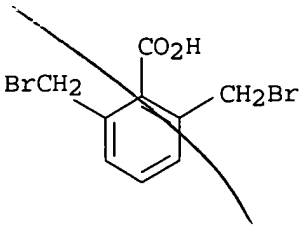
AB A new binuclear Cu(II) complex, [Cu2L.Br2]Br·H2O, where L is a new binucleating macrocyclic ligand 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoate, was prepared and characterized by x-ray crystallog. Crystal data: monoclinic, space group P21/c, a 1.1666(2), b 1.3541(3), c 2.2750(5) nm, β 99.38(3)°, Z = 4. The binuclear Cu(II) center ions are bridged by a μ-carboxyl group of L and separated by 0.5884 nm. Both of the Cu(II) ion centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one O of the carboxyl group, as well as one bromide ion. The Cu(II) ion is in the trigonal bipyramid environment. Variable temperature magnetic susceptibility studies indicate that there exists intramol. antiferromagnetic coupling (J = -22.49cm-1) between the two Cu(II) centers.

IT **56263-54-8**, 2,6-Bis(bromomethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of copper bis(triazacyclododecanylmethyl)benzoate dinuclear complex)

RN 56263-54-8 CAPLUS

10803578

CN Benzoic acid, 2,6-bis(bromomethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 34 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:271373 CAPLUS
DN 130:282365
TI Coding combinatorial libraries with fluorine tags
IN Hochlowski, Jill E.; Sowin, Thomas J.; Norbeck, Daniel W.; Wade, Warren S.; Whittern, David N.
PA Abbott Laboratories, USA
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

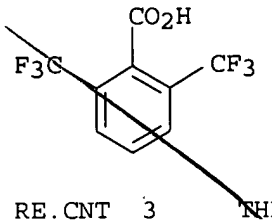
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9919344	A1	19990422	WO 1998-US21408	19981009
	W: CA, JP, MX				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6168913	B1	20010102	US 1997-949987	19971014
	CA 2305771	AA	19990422	CA 1998-2305771	19981009
	EP 1023317	A1	20000802	EP 1998-953379	19981009
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2001519439	T2	20011023	JP 2000-515915	19981009
PRAI	US 1997-949987	A	19971014		
	WO 1998-US21408	W	19981009		

AB The present invention relates to coding combinatorial chemical libraries synthesized on a plurality of solid supports by attaching "tags" that comprise fluorine containing compds. in combinations and/or ratios. The tags can be decoded while attached to the solid support by fluorine NMR spectroscopy to follow the reaction history of individual beads, and to determine the particular member of the library that is attached on the bead. Thus, coupling of Boc-Lys(Fmoc)-OH (Boc = Me3CO2C; Fmoc = 9-fluorenylmethoxycarbonyl) to (aminomethyl)polystyrene, followed by Fmoc deprotection and attachment of fluorine tag 3-(4-fluorophenyl)propionic acid gave tagged resin with a 19F NMR peak at -118 ppm. Other resins containing 3,5-difluorophenylacetic acid, 4-(trifluoromethyl)benzoic acid, and 4-(trifluoromethoxy)benzoic acid were prepared, and showed 19F NMR peaks at -110, -63, and -58 ppm, resp. The tagged resins were split and pooled in defined coding ratios, linker 4-[4-(hydroxymethyl)phenoxy]butyric acid attached, and a coded, Fmoc-protected amino acid residue attached. The resins were pooled and split again, followed by deprotection and sulfonylation with alkyl and aromatic sulfonyl chlorides. The resulting sulfonated amino acid resins were pooled and split a third time, followed by deprotonation and alkylation with alkyl bromides. Addnl. methods for attaching fluorine labels to solid-phase synthesis resins are also described.

IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(coding combinatorial libraries with fluorine tags)

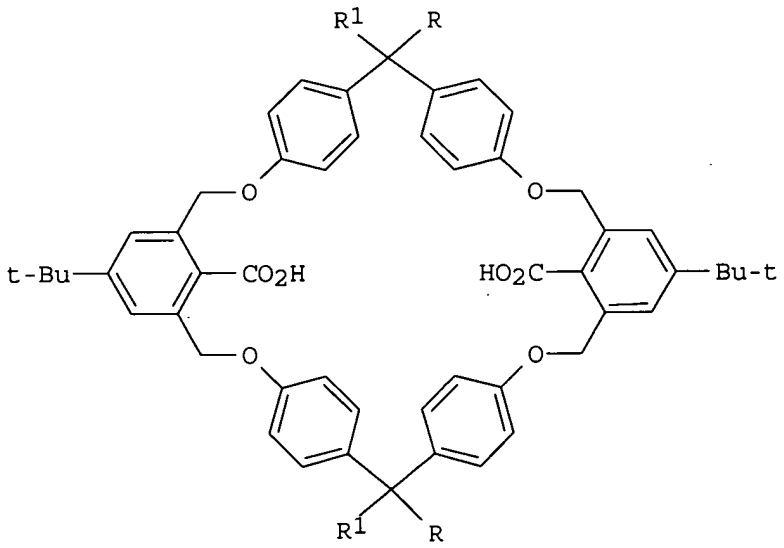
10803578

RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:255217 CAPLUS
DN 131:44803
TI Preorganized macrocyclic receptors featuring endo-carboxylic acid groups. Host synthesis and inclusion compounds with alcohol and amine guests
AU Weber, Edwin; Haase, Reinhard; Pollex, Rolf; Czugler, Matyas
CS Institut Organische Chemie, Technische Universitat-Bergakademie Freiberg, Freiberg, D-09596, Germany
SO Journal fuer Praktische Chemie (Weinheim, Germany) (1999), 341(3), 274-283
CODEN: JPCHF4; ISSN: 1436-9966
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 131:44803
GI



I

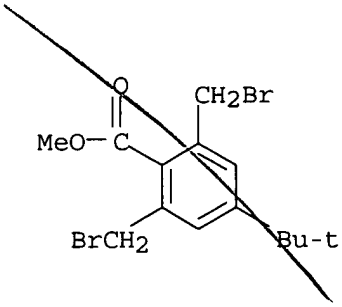
AB The synthesis and characterization of macrocyclic host compds. I [RR1 = (CH2)5; R, R1 = Me; RR1 = O; R = Me, R1 = CH2CO2H] having modified diphenylmethane units as bridging elements and 2 endo-oriented carboxyl groups attached to aromatic building blocks are described. The complexation properties of the macrocycles towards amines and alcs. are reported, showing that the ability to form convergent inclusion compds. depends on

the type of the spacer element. For the dicarboxylic hosts I [RR1 = (CH2)5; R, R1 = Me] endo-complexation of guest mols. based on H bonding to the acid functions is proved using 1H NMR and x-ray crystal structure anal.

IT **119319-00-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of preorganized macrocyclic receptors with endo-carboxyl groups)

RN 119319-00-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)

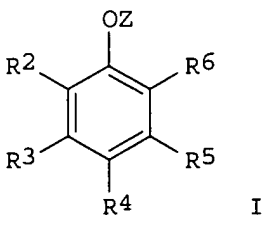


RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

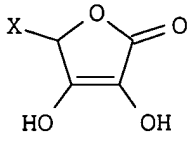
L3 ANSWER 36 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:157080 CAPLUS
DN 130:229933
TI Silver halide photographic material, photography, and processing thereof
IN Ho, Sokuman
PA Konica Co., Japan
SO Jpn. Kokai Tokkyo Koho, 44 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 11065014	A2	19990305	JP 1997-223555	19970820
PRAI JP 1997-223555		19970820		

GI



I



II

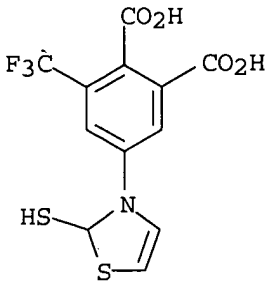
AB The title material, possessing a Ag halide emulsion layer on a support, is chemical sensitized in the presence of ≥1 compound RSMm (R = aliphatic, aromatic, heterocyclic or alicyclic group substituted by water-soluble groups; M
= H, alkali metal, cation; m = 0 or 1, when m = 0, the compound has the formula R:S) and contains a developing agent I (R2-6 = H or substituent,

the total C number of R2-6 is ≥8 and ≥1 of R2 and R4 is OH, sulfonamide or carbonamide, R2-6 may form a ring along with OZ ; Z = H or protective group which is released under alkali conditions to form OH) or II (X = aryl, heterocyclic group, CR11R12R13; R11-13 = H or substituent other than OH). The title processing method includes development, fixing, and drying steps, in which the total processing time is ≤60 s and the replenishment rate of the developing and fixing solns. is ≤30 cc/10 + 12 in. size. A photog. method is also claimed, in which the material sandwiched between high-sensitive intensifying screens in which the filling rate of the fluorescent substance is 68-90% is subjected to x-ray photograph. The material, useful as a medical x-ray film, shows low fog, high sensitivity, decreased residual color stain, and improved storage stability.

IT **221072-53-3**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(photog. emulsion chemical sensitized in presence of sulfur compound fog inhibitor)

RN 221072-53-3 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 5-(2-mercapto-3(2H)-thiazolyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 37 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:68332 CAPLUS

DN 130:296671

TI Preorganized macrocyclic dicarboxylic receptors: Synthesis, inclusion behavior and structural study

AU Pollex, Rolf; Weber, Edwin; Czugler, Matyas

CS Institut fur Organische Chemie, Technische Universitat Bergakademie Freiberg, Freiberg/Sa., D-09596, Germany

SO Molecular Recognition and Inclusion, Proceedings of the International Symposium on Molecular Recognition and Inclusion, 9th, Lyon, Sept. 7-12, 1996 (1998), Meeting Date 1996, 467-470. Editor(s): Coleman, Annette W. Publisher: Kluwer, Dordrecht, Neth.
CODEN: 67FSAY

DT Conference

LA English

AB The authors report here synthesis, inclusion behavior and structural study of preorganized macrocyclic dicarboxylic receptors.

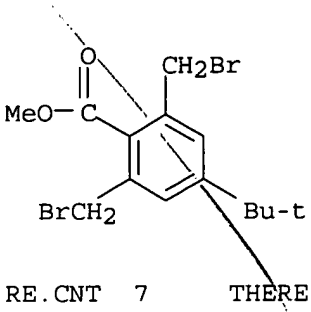
IT **119319-00-5**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(synthesis, inclusion behavior and structural study of preorganized macrocyclic dicarboxylic receptors)

RN 119319-00-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester

10803578

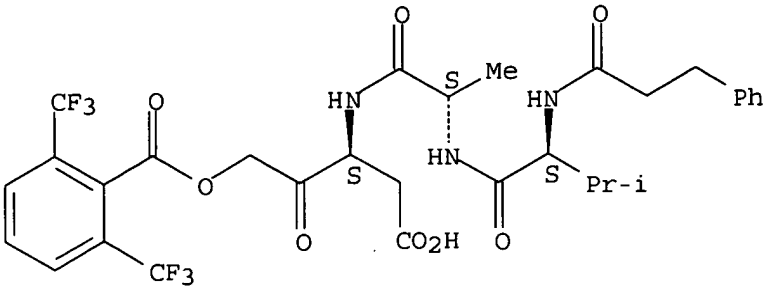
(9CI) (CA INDEX NAME)



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:59441 CAPLUS
DN 130:261459
TI Three-Dimensional Quantitative Structure-Activity Relationship of Interleukin 1-β Converting Enzyme Inhibitors: A Comparative Molecular Field Analysis Study
AU Kulkarni, Santosh S.; Kulkarni, Vithal M.
CS Department of Chemical Technology Pharmaceutical Division, University of Mumbai, Mumbai, 400 019, India
SO Journal of Medicinal Chemistry (1999), 42(3), 373-380
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB A three-dimensional quant. structure-activity relationship (QSAR) study using the comparative mol. field anal. (CoMFA) method was performed on a series of interleukin 1-β converting enzyme (ICE) inhibitors. The compds. studied have been reported to be time-dependent inhibitors of ICE. This study was performed using 49 compds., in which the CoMFA models were developed using a training set of 39 compds. All the compds. were modeled using the X-ray crystal structure of tetrapeptide aldehyde inhibitor/ICE complex. The inhibitor compds. were considered both as neutral species and as P1 carboxylate ionized species. Superimpositions were performed using two alignment rules, namely, an alignment of the structures based on RMS fitting of the backbone heavy atoms of each structure to compound 2 and an alignment based on SYBYL QSAR rigid body field fit of the steric and electrostatic fields of the mols. to the fields of compound 2. Use of LUMO energies or ClogP as addnl. descriptors in the QSAR table did not improve the significance of the CoMFA models. Steric and electrostatic fields of the inhibitors were found to be the relevant descriptors for structure-activity relationships. The predictive ability of the CoMFA model was evaluated by using a test set of 10 compds. (r2pred as high as 0.859). Further comparison of the coefficient contour maps with the steric and electrostatic properties of the receptor show a high level of compatibility.
IT **151272-16-1 154674-82-5 154719-26-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR of interleukin 1β converting enzyme inhibitors: comparative mol. field anal. study)
RN 151272-16-1 CAPLUS
CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

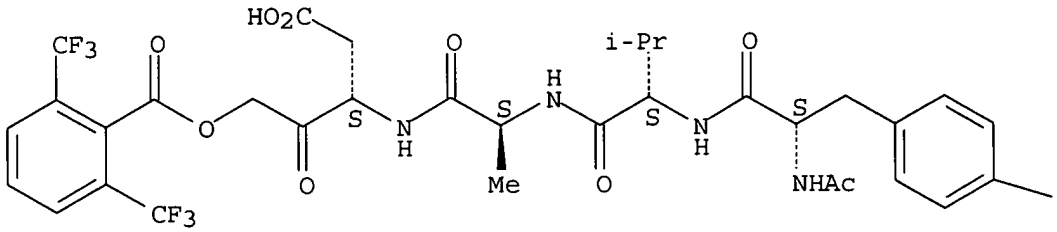
Absolute stereochemistry.



RN 154674-82-5 CAPLUS
CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

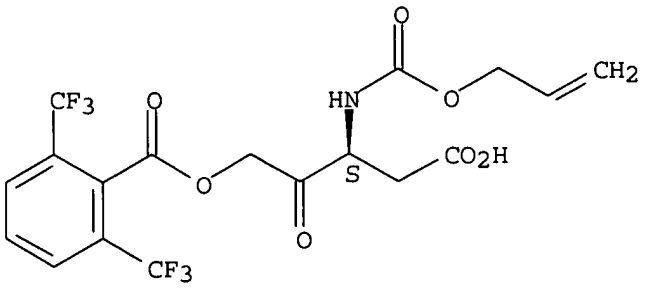


PAGE 1-B

—OH

RN 154719-26-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (3S)-4-carboxy-2-oxo-3-[[(2-propenyloxy)carbonyl]amino]butyl ester (9CI) (CA INDEX NAME)

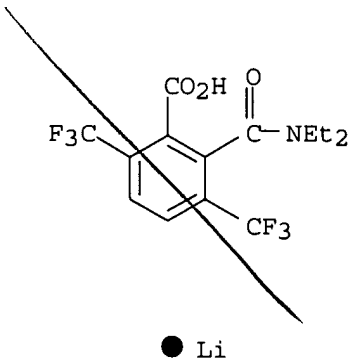
Absolute stereochemistry.



10803578

RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

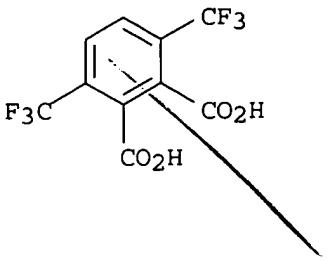
L3 ANSWER 39 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:648841 CAPLUS
DN 129:350160
TI Oxygen atom transfer from μ-Oxobis[1,4,8,11,15,18,22,25-octakis(trifluoromethyl)phthalocyaninato]diiron(III): Evidence for an FeIV=O intermediate
AU Chen, Michael J.; Fremgen, David E.; Rathke, Jerome W.
CS Chemical Technology Division, Argonne National Laboratory, Argonne, IL, 60439, USA
SO Journal of Porphyrins and Phthalocyanines (1998), 2(6), 473-482
CODEN: JPPHFZ; ISSN: 1088-4246
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB The dimeric complex [(FPc)Fe]2(μ-O) (1, FPc is the dianion of 1,4,8,11,15,18,22,25-octakis(trifluoromethyl)phthalocyanine) was shown to transfer its μ-oxo atom quant. to trimethylphosphine and triphenylphosphine. In the case of triphenylphosphine a base such as 1-methylimidazole (MeIm) or pyridine (py) is needed to induce the oxygen atom transfer. The reaction of 1 with MeIm at -40° and below gives [(MeIm)(FPc)Fe]2(μ-O) (4), which disproportionates to give (MeIm)2(FPc)Fe (5) and (FPc)Fe:O (6) at higher temps. The oxo atom of 6 was shown to transfer to triphenylphosphine. Similarly, 6 is generated by the disproportionation of 1 with py. It also was generated by the oxidation of 1 with t-Bu hydroperoxide. [(FPc)Fe]2(μ-O) catalyzes the oxidation of hydrocarbons by iodosylbenzene. With stilbenes, styrenes, cyclohexenes and butenes as substrates, both epoxidn. and alkyl C-H bond oxidns. were observed The epoxidn. of cis-stilbene leads to a mixture of cis- and trans-stilbene oxides, indicating that epoxidn. of cis-stilbene, and possibly other olefins as well, proceeds through a non-concerted mechanism.
IT **215382-68-6P**, Lithium 3,6-bis(trifluoromethyl)-2-(N,N-diethylamido)benzoate **215382-70-0P**, Lithium 3,6-bis(trifluoromethyl)phthalate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of iron octakis(trifluoromethyl)phthalocyaninato oxo-bridged dinuclear complex)
RN 215382-68-6 CAPLUS
CN Benzoic acid, 2-[(diethylamino)carbonyl]-3,6-bis(trifluoromethyl)-, lithium salt (9CI) (CA INDEX NAME)



RN 215382-70-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)-, dilithium salt

10803578

(9CI) (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 40 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:568911 CAPLUS
DN 129:184238
TI Screening for thymocyte caspase activity modulators
IN Reinherz, Ellis; Clayton, Linda; Ocain, Timothy D.; Patch, Raymond J.
PA Dana Farber Cancer Institute, USA; Procept, Inc.
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9836057	A1	19980820	WO 1998-US3524	19980217
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI	US 1997-802474	A	19970218		
	US 1997-948124	A	19971009		

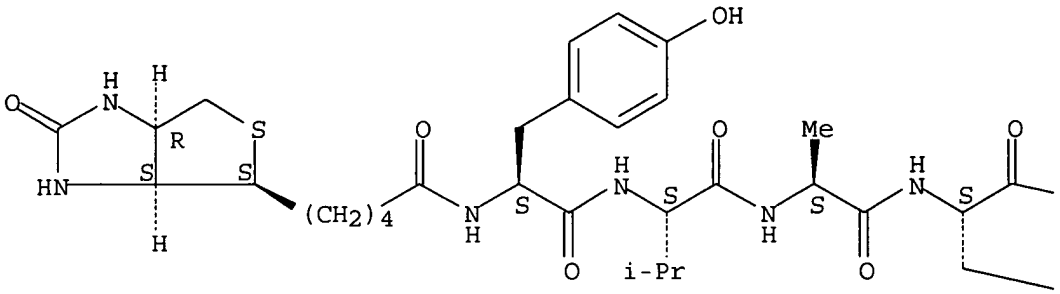
AB Work described herein shows that T cell receptor triggering by peptide/MHC ligands activates a caspase in thymocytes, including CD4+CD8+ double pos. thymocytes, resulting in their death. Methods of inhibiting apoptosis in thymocytes are described, as well as assays for identifying an agent which alters the activity of the caspase are described.

IT **211918-96-6P 211919-00-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(screening for thymocyte caspase activity modulators)

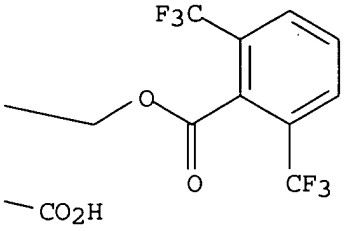
RN 211918-96-6 CAPLUS
CN L-Alaninamide, N-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



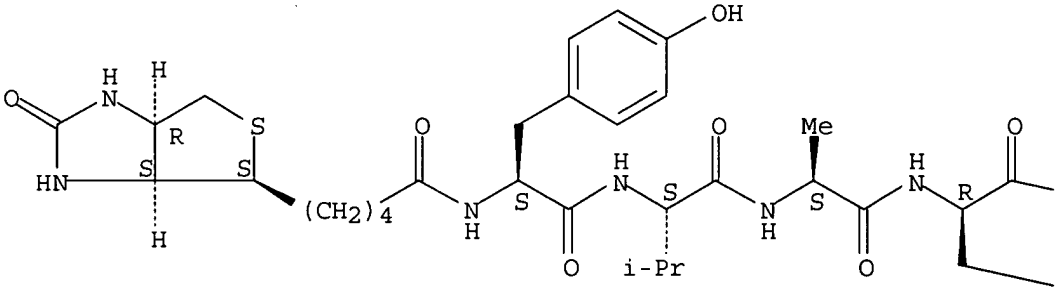
PAGE 1-B

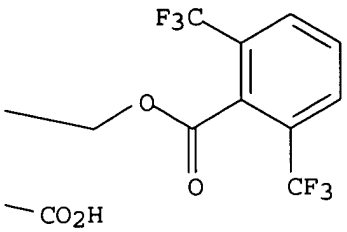


RN 211919-00-5 CAPLUS
CN L-Alaninamide, N-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-tyrosyl-L-valyl-N-[(1R)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

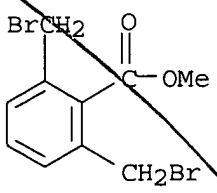
PAGE 1-A





RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 41 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:536846 CAPLUS
DN 129:260442
TI Uranyl binding by a novel bis-calix[4]arene receptor
AU Schmitt, Philippe; Beer, Paul D.; Drew, Michael G. B.; Sheen, Paul D.
CS Inorg. Chem. Lab., Univ. Oxford, Oxford, OX1 3QR, UK
SO Tetrahedron Letters (1998), 39(35), 6383-6386
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
AB A new bis-calix[4]arene receptor has been synthesized which complexes and exts. the uranyl cation in organic media. The two halves of the bis-calix[4]arene are connected by two (2-carboxy-m-phenylene)dimethylene units.
IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(uranyl binding by bis-calix[4]arene receptor)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

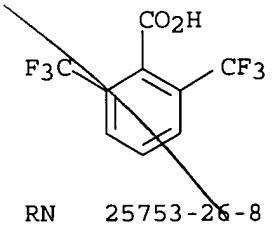


RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

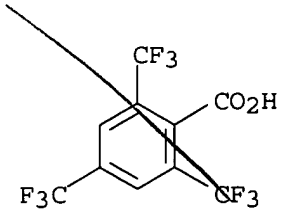
L3 ANSWER 42 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:482605 CAPLUS
DN 129:189002
TI Bis- and oligo(trifluoromethyl)benzenes: hydrogen/metal exchange rates and gas-phase acidities
AU Schlosser, Manfred; Mongin, F.; Porwisiak, Jacek; Dmowski, Wojciech; Buker, Heinz H.; Nibbering, Nico M. M.
CS Institut de Chimie organique de l'Universite, Lausanne-Dorigny, CH-1015, Switz.
SO Chemistry--A European Journal (1998), 4(7), 1281-1286
CODEN: CEUJED; ISSN: 0947-6539

10803578

PB Wiley-VCH Verlag GmbH
DT Journal
LA English
AB The proton mobilities (kinetic acidities) of bis- and tris(trifluoromethyl)benzene are dictated to a large extent by steric factors; the trifluoromethyl group is a fairly bulky substituent that can seriously impede the approach of the metalating reagent. Most satisfactory results in terms of yields and selectivities have been achieved with lithium 2,2,6,6-tetramethylpiperidide or with methyllithium in the presence of potassium tert-butoxide, a slim version of the standard superbase. The rates of deprotonation under irreversible conditions do not parallel the thermodn. (equilibrium) acidities. Substituent effects on the deprotonation energies in the gas phase appear to be additive: each trifluoromethyl group lowers it by 13 kcal mol-1 when located ortho with respect to the carbanion, and by 10 kcal mol-1 when located in a meta or para position.
IT **24821-22-5P**, 2,6-Bis(trifluoromethyl)benzoic acid
25753-26-8P, 2,4,6-Tris(trifluoromethyl)benzoic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrogen/metal exchange rates and gas-phase acidities of bis- and oligo(trifluoromethyl)benzenes)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 25753-26-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



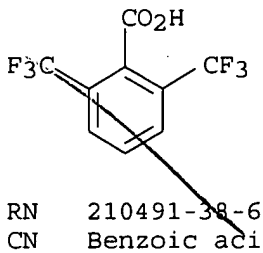
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 43 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:344782 CAPLUS
DN 129:135946
TI A site selective functionalization of 1,3-bis(trifluoromethyl)benzene
AU Dmowski, Wojciech; Piasecka-Maciejewska, Krystyna
CS Institute Organic Chemistry, Polish Academy Sciences, Warsaw, 01-224, Pol.
SO Tetrahedron (1998), 54(24), 6781-6792
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 129:135946
AB 1,3-Bis(trifluoromethyl)benzene was regioselectively metalated and subsequently carboxylated at position 2 to give 2,6-

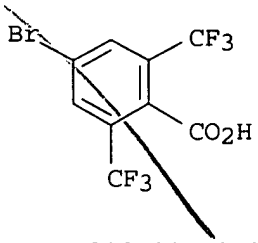
bis(trifluoromethyl)benzoic acid. Treatment of the acid with sulfur tetrafluoride gave 2,6-bis(trifluoromethyl)benzyl fluoride which was readily converted to 2,6-bis(trifluoromethyl)benzyl alc. and further to 2,6-bis(trifluoromethyl)benzaldehyde. Bromination of 2,6-bis(trifluoromethyl)benzoic acid with 1,1-dibromo-5,5-dimethylhydantoin proceeded regioselectively affording 4-bromo-2,6-bis(trifluoromethyl)benzoic acid almost quant. The latter was fluorinated to the corresponding acid fluoride which on treatment with methanolic sodium methoxide gave 4-methoxy-2,6-bis(trifluoromethyl)benzoic acid or its Me ester, depending on the reaction conditions. 4-Methoxy-2,6-bis(trifluoromethyl)benzoic acid, via its acid fluoride, was also transformed, first to the corresponding benzyl alc., then to the benzaldehyde. Lithiation of 4-methoxy-2,6-bis(trifluoromethyl)benzoic acid, followed by methylation, proceeded with low selectivity, nevertheless, Me 4-methoxy-3-methyl-2,6-bis(trifluoromethyl)benzoate was formed as the main product which was stepwise converted to 4-methoxy-3-methyl-2,6-bis(trifluoromethyl)benzyl alc. and 4-methoxy-3-methyl-2,6-bis(trifluoromethyl)benzaldehyde, albeit in low total yield.

IT **24821-22-5P 210491-38-6P 210491-41-1P 210491-43-3P 210491-44-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(site- selective functionalization of bis(trifluoromethyl)benzene)

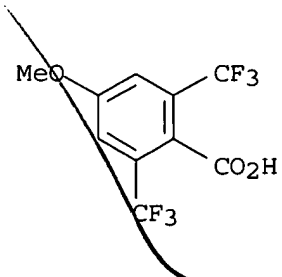
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 210491-38-6 CAPLUS
CN Benzoic acid, 4-bromo-2,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

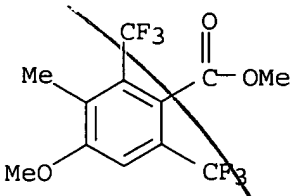


RN 210491-41-1 CAPLUS
CN Benzoic acid, 4-methoxy-2,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

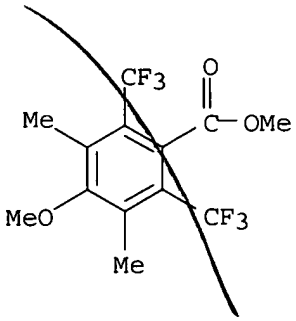


RN 210491-43-3 CAPLUS
CN Benzoic acid, 4-methoxy-3-methyl-2,6-bis(trifluoromethyl)-, methyl ester

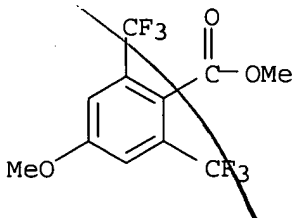
(9CI) (CA INDEX NAME)



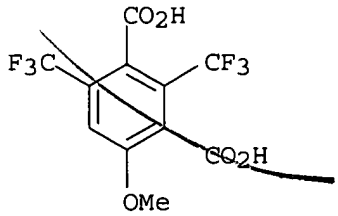
RN 210491-44-4 CAPLUS .
CN Benzoic acid, 4-methoxy-3,5-dimethyl-2,6-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



IT **210491-40-0P 210491-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(site- selective functionalization of bis(trifluoromethyl)benzene)
RN 210491-40-0 CAPLUS
CN Benzoic acid, 4-methoxy-2,6-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 210491-42-2 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-methoxy-2,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 44 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:330458 CAPLUS
DN 129:81939

10803578

TI The design and synthesis of inhibitors of the cysteinyl protease, Der p I

AU Billson, Jeremy; Clark, Jonathan; Conway, Simon P.; Hart, Terance; Johnson, Tony; Langston, Steven P.; Ramjee, Manoj; Quibell, Martin; Scott, Richard K.

CS Peptide Therapeutics Group plc, The Cambridge Science Park, Cambridge, CB4 4WG, UK

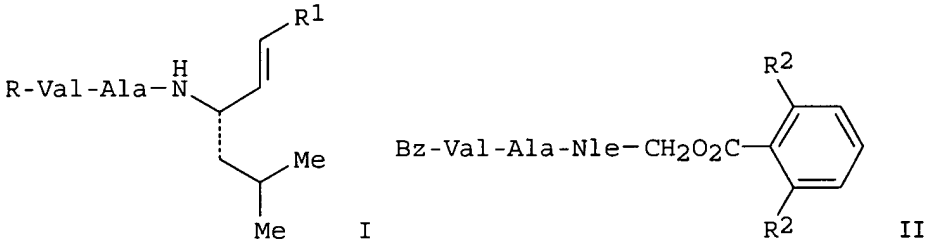
SO Bioorganic & Medicinal Chemistry Letters (1998), 8(9), 993-998
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

GI



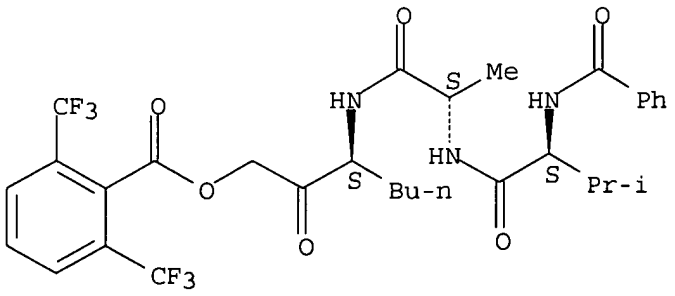
AB Prototype irreversible inhibitors I [R = H, Me3CO2C (Boc), Ac, Bz, R1 = CO2Et; R = Boc, R1 = SO2Me, SO2CH2Ph, SO2Ph] and II (R2 = H, Me, Cl, CF3) of the cysteinyl protease Der p I were designed, synthesized and evaluated in vitro. Candidates were designed using a modular approach, whereby a peptide sequence was appended with known thiophilic moieties. This hinged on utilizing peptide sequences from substrate specificity data compiled using proprietary RAPiD technol.

IT **187991-44-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design and synthesis of cysteinyl protease Der p I inhibitors)

RN 187991-44-2 CAPLUS

CN L-Alaninamide, N-benzoyl-L-valyl-N-[(1S)-1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(design and synthesis of cysteinyl protease Der p I inhibitors)

RN 24821-22-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

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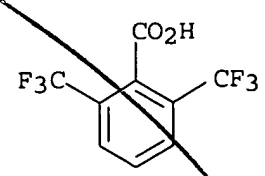
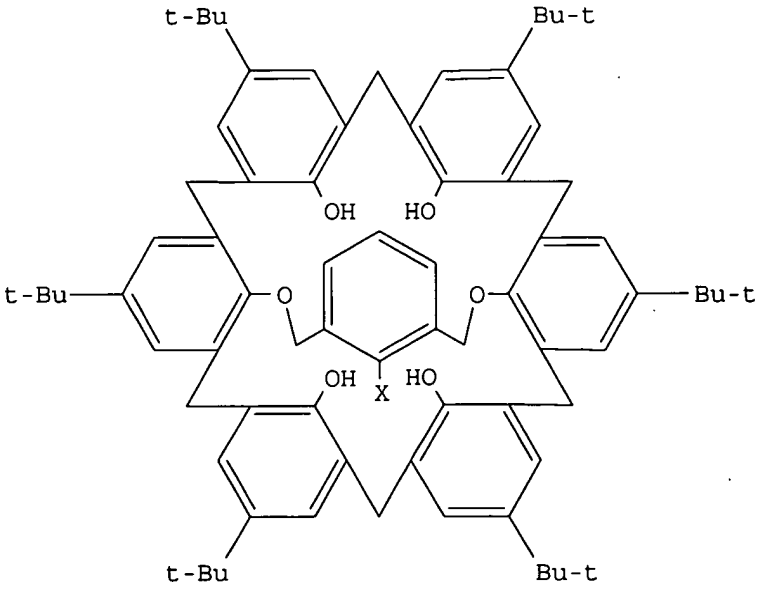


RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 45 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:322978 CAPLUS
DN 129:53992
TI Concave reagents. Part 27. Steric requirements of intraannular substituents in A,D-bridged calix[6]arenes
AU Luning, Ulrich; Ross, Haymo; Thondorf, Iris
CS Institut fur Organische Chemie, Christian-Albrechts-Universitat zu Kiel, Kiel, D-24098, Germany
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1998), (6), 1313-1317
CODEN: JCPKBH; ISSN: 0300-9580
PB Royal Society of Chemistry
DT Journal
LA English
GI



I

AB A series of A,D-m-xylylene bridged calix[6]arenes I carrying substituents of different size in 2-position of the bridge have been investigated by dynamic NMR spectroscopy and by force field methods. Mol. mechanics calcns. indicate a bean shaped conformation as the global energy min. in which the calixarene scaffold adopts a half-pinched/half-winged arrangement.

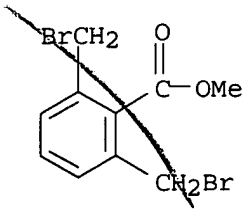
IT **56263-51-5**, Methyl 2,6-bis(bromomethyl)benzoate

10803578

RL: RCT (Reactant); RACT (Reactant or reagent)
(steric requirements of intraannular substituents in A,D-bridged calix[6]arenes)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 46 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:255296 CAPLUS

DN 129:4637

TI Synthesis of novel water-soluble molecular bowls and their unique complexing behavior with 1-anilinonaphthalene-8-sulfonate

AU Goto, Kei; Akine, Shigehisa; Hayashi, Tomoko; Okazaki, Renji

CS Department of Chemistry, Graduate School of Science, The University of Tokyo, Tokyo, 113, Japan

SO Chemistry Letters (1998), (4), 291-292
CODEN: CMLTAG; ISSN: 0366-7022

PB Chemical Society of Japan

DT Journal

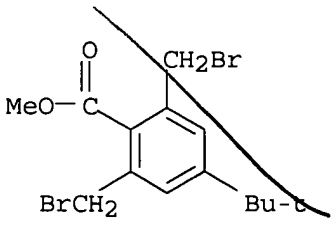
LA English

AB Novel water-soluble bowl-shaped cyclophanes were synthesized. Complexation study in 25% aqueous methanol revealed that the bowl-shaped cyclophanes form 2:1 (host/guest) complexes with 1-anilinonaphthalene-8-sulfonate (ANS). The emission wavelength of ANS encapsulated by bowl-shaped cyclophanes as well as the related monocyclic cyclophanes was usefully employed to demonstrate that the host/guest ratio of the complex significantly affects the micropolarity of the guest-binding site of these cyclophanes.

IT **119319-00-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of water-soluble bowl-shaped cyclophanes and their complexing behavior with anilinonaphthalenesulfonate)

RN 119319-00-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 47 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

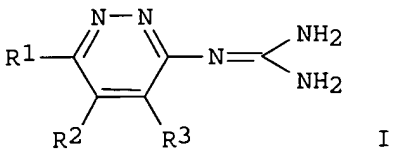
AN 1998:163375 CAPLUS

10803578

DN 128:204895
TI Preparation of pyridazinylguanidines as sodium-hydrogen exchange inhibitors
IN Shiraishi, Mitsuru; Imamiya, Eiko; Kusumoto, Keiji; Ichimori, Yuzo
PA Takeda Chemical Industries, Ltd., Japan
SO Eur. Pat. Appl., 59 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 825187	A1	19980225	EP 1997-114342	19970820
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	CA 2213594	AA	19980222	CA 1997-2213594	19970821
	JP 10114753	A2	19980506	JP 1997-224945	19970821
PRAI	JP 1996-221553	A	19960822		

OS MARPAT 128:204895
GI

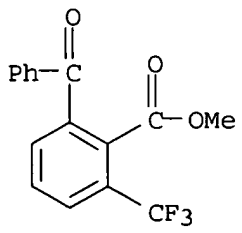


I

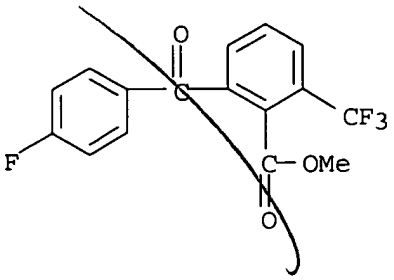
AB Title compds. [I; R1 = (un)substituted aromatic ring group (sic); R2R3 = atoms to complete an (un)substituted fused (N-containing) aromatic ring] were prepared Thus, 2,6-I(PhCO)C6H3CO2Me was cyclocondensed with H2NNH2 and the chlorinated product condensed with guanidine to give I (R1 = Ph, R2R3 = CH:CHCH:CI). Data for biol. activity of I were given.

IT **203729-28-6P 203729-66-2P 203729-80-0P 203729-91-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridazinylguanidines as sodium-hydrogen exchange inhibitors)

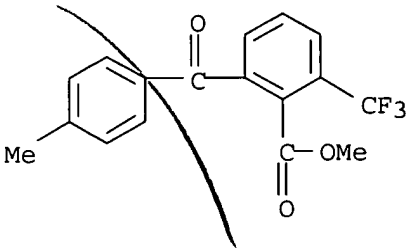
RN 203729-28-6 CAPLUS
CN Benzoic acid, 2-benzoyl-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



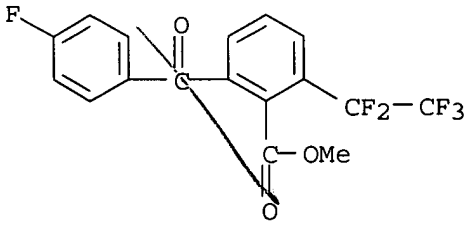
RN 203729-66-2 CAPLUS
CN Benzoic acid, 2-(4-fluorobenzoyl)-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 203729-80-0 CAPLUS
CN Benzoic acid, 2-(4-methylbenzoyl)-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 203729-91-3 CAPLUS
CN Benzoic acid, 2-(4-fluorobenzoyl)-6-(pentafluoroethyl)-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 48 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:121460 CAPLUS
DN 128:217140
TI Preparation and reactions of 2,4,6-tris(trifluoromethyl)phenylamine
AU Ahlemann, Jens-T.; Roesky, Herbert W.; Noltemeyer, Mathias; Schmidt, Hans-G.; Markovsky, Leonid N.; Shermolovich, Yuri G.
CS Tammannstrasse 4, Institut fur Anorganische Chemie der Georg-August-Universitat Gottingen, Gottingen, 37077, Germany
SO Journal of Fluorine Chemistry (1998), 87(1), 87-90
CODEN: JFLCAR; ISSN: 0022-1139
PB Elsevier Science S.A.
DT Journal
LA English
OS CASREACT 128:217140
AB Starting from RfH [Rf = 1,3,5-tris(trifluoromethyl)phenyl], RfNH2 is obtained in a four-step synthesis. RfNH2 reacts with chlorotrimethylsilane in the presence of DBU forming the mono- and bis-silylated amines RfNHSiMe3 and RfN(SiMe3)2. The potassium salt of

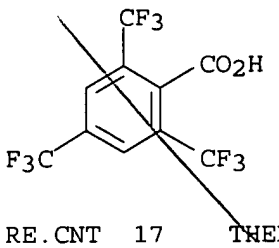
10803578

RfNHSiMe3 reacts with SiCl4 yielding RfN(SiCl3)2.

IT **25753-26-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of tris(trifluoromethyl)phenylamine)

RN 25753-26-8 CAPLUS

CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 49 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:77165 CAPLUS
Correction of: 1998:77167

DN 128:267567
Correction of: 128:267521

TI Docking of a series of peptide-based interleukin-1β converting enzyme inhibitors with aspartyl hemiacetals, α-((2,6-dichlorobenzoyl)oxy)methyl and (acyloxy)methyl ketone moieties

AU Hariprasad, Vankayalapati; Kulkarni, Vithal M.

CS Pharmaceutical Division, University of Mumbai, Mumbai, 400019, India

SO Journal of Molecular Modeling [Electronic Publication] (1997), 3(10), 443-454
CODEN: JMMOFK; ISSN: 0948-5023
URL: http://link.springer.de/link/service/journals/00894/bibs/7003010/70030443.htm

PB Journal of Molecular Modeling

DT Journal; (online computer file)

LA English

AB The enzyme-binding mode of a series of interleukin-1β converting enzyme (ICE) inhibitors has been analyzed on the basis of the crystal structure of the complex between hICE (human ICE) and tetrapeptide aldehyde. The conformation adopted by these inhibitors was very similar to and could be superimposable onto the regions of crystal structure. The active and the low energy conformers were docked either by grid or manually into the binding site. The anal. of the resulting model indicated that O-benzylacyl group of aspartyl hemiacetals interact with Cys285; the series of large substituents [such as semicarbazone, 2,6-bis(trifluoromethyl)benzoate, and α-[(2,6-dichlorobenzoyl)oxy]methyl ketone, etc.] of P1 site protrude from the surface of Cys285 and interact with Val338, which is located below the binding pocket. The hydrogen bonding interaction between NH of semicarbazone and Cys285 seems to have significant role. The total potential energy including intermol. interaction energy, consisting of van der Waals and electrostatic energies were calculated The resulting model is qual. consistent with the reported exptl. data and can be useful for the design of more potent inhibitors of ICE.

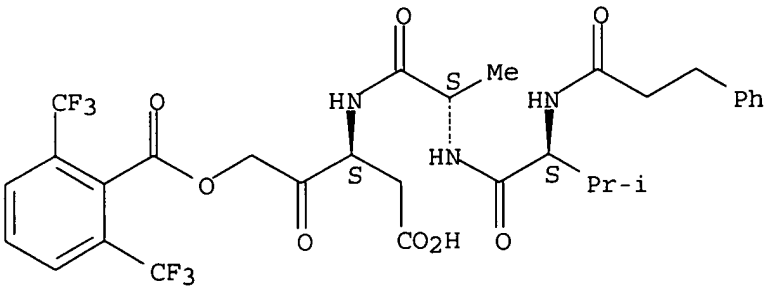
IT **151272-16-1 154674-82-5 154719-26-3**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(docking anal. of peptide-based interleukin-1β converting enzyme

inhibitors)

RN 151272-16-1 CAPLUS

CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

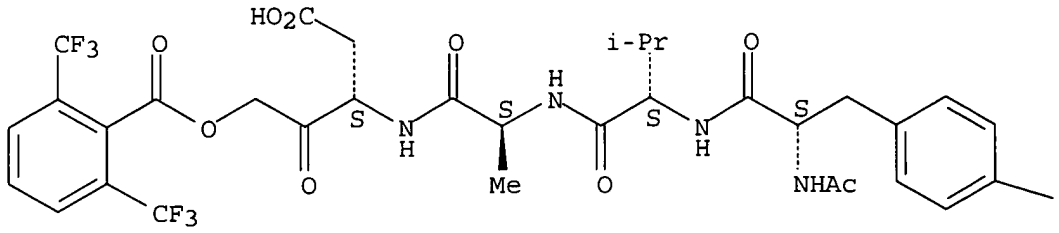


RN 154674-82-5 CAPLUS

CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



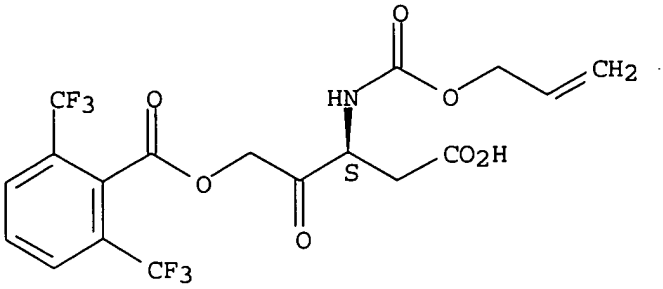
PAGE 1-B

—OH

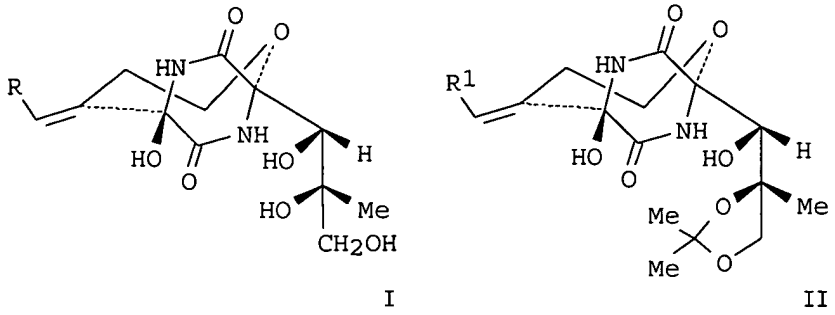
RN 154719-26-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (3S)-4-carboxy-2-oxo-3-[[(2-propenyloxy)carbonyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 50 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:74194 CAPLUS
DN 128:167286
TI 5a-Methyl-Substituted Bicyclomycins: Synthesis and Chemical, Biochemical, and Biological Properties
AU Santillan, Alejandro, Jr.; Zhang, Xiangdong; Widger, William R.; Kohn, Harold
CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
SO Journal of Organic Chemistry (1998), 63(4), 1290-1298
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
GI



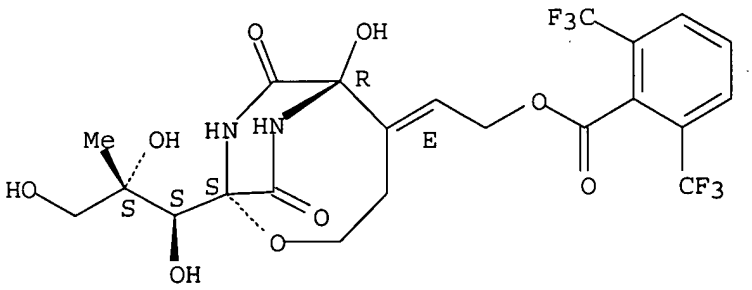
I II

AB A select series of 5a-methyl-substituted bicyclomycins I [R = Me, CH2OH, CH2OAc, CH2O2CC6H3(CF3)2-2,6, CH2Cl, CH2Br, CH2N3, CH2NH2, CH2NHAc, CH2SEt] were prepared to identify interactions that influence antibiotic binding to the Escherichia coli rho transcription termination factor and to aid in identifying the bicyclomycin binding domain. The regioselective reduction of Me 5a-bicyclomycincarboxylate C(2'),C(3')-acetonide (II; R1 = CO2Me) using lithium triethylborohydride provided 5a-(hydroxy)methylbicyclomycin C(2'),C(3')-acetonide (II; R1 = CH2OH). Alc. II (R1 = CH2OH) served as the key synthetic intermediate in preparing the targeted compds. Replacing or modifying the terminal hydroxy group in II (R1 = CH2OH) gave the corresponding hydrogen, acyl, halogen, azide, amine, and amide derivs., which were then treated with trifluoroacetic acid to remove the C(2'),C(3')-acetonide protecting group to give 2-10. The chemical reactivity of 5a-(chloromethyl)bicyclomycin [I; R = CH2Cl (III)] with the nucleophile EtSH was compared with bicyclomycin [I; R = H (IV)]. It was found that allylic chloride III underwent SN2 displacement with EtSH, while IV furnished C(5)-C(5a) exomethylene group modified adducts,

suggesting that III may serve as a site selective irreversible alkylation probe. Evaluation of I in rho functional assays showed that 5a-methylbicyclomycin (I; R = Me), 5a-(hydroxy)methylbicyclomycin (I; R = CH2OH), 5a-[2,6-bis-(trifluoromethyl)benzoxy]methylbicyclomycin [I; R = CH2O2CC6H3(CF3)2-2,6], 5a-(azido)methylbicyclomycin (I; R = CH2N3), 5a-(ethylmercapto)methylbicyclomycin (I; R = CH2SEt), and III all exhibited inhibitory properties comparable with IV. The activities of these compds. and the remaining bicyclomycins within this series provided information of the structural interactions that occur with drug binding. Finally, we found that I (R = Me) displayed comparable antimicrobial activity with IV in the filter disk assay. Compound I (R = Me) is the most biol. active bicyclomycin derivative reported to date.

IT **202730-09-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, chemical, biochem., and biol. properties of 5a-methyl-substituted bicyclomycins)
RN 202730-09-4 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-[6-hydroxy-8,10-dioxo-1-(1,2,3-trihydroxy-2-methylpropyl)-2-oxa-7,9-diazabicyclo[4.2.2]dec-5-ylidene]ethyl ester, [1S-[1α(1R*,2R*),5E,6β]]- (9CI) (CA INDEX NAME)

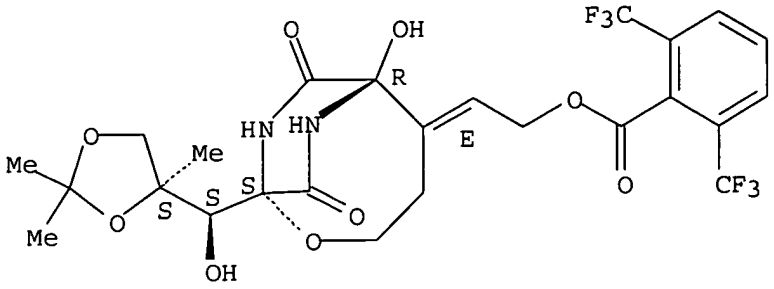
Absolute stereochemistry.
Double bond geometry as shown.



IT **202730-32-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, chemical, biochem., and biol. properties of 5a-methyl-substituted bicyclomycins)
RN 202730-32-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-[6-hydroxy-1-[hydroxy(2,2,4-trimethyl-1,3-dioxolan-4-yl)methyl]-8,10-dioxo-2-oxa-7,9-diazabicyclo[4.2.2]dec-5-ylidene]ethyl ester, [1S-[1α[R*(R*)],5E,6β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

10803578

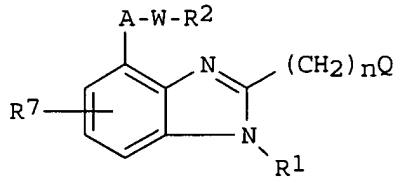


RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 51 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:65895 CAPLUS
DN 128:102090
TI Preparation of novel benzimidazole derivatives for treatment of acidophilia, bronchial asthma, and allergic disease
IN Mizuguchi, Kiyoshi; Ohzawa, Nobuo; Nakai, Yasuhiro; Matsuura, Kazuyuki; Ohnishi, Shuhei
PA Mochida Pharmaceutical Co., Ltd., Japan; Mizuguchi, Kiyoshi; Ohzawa, Nobuo; Nakai, Yasuhiro; Matsuura, Kazuyuki; Ohnishi, Shuhei
SO PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9801429	A1	19980115	WO 1997-JP2308	19970703
	W: CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2259585	AA	19980115	CA 1997-2259585	19970703
	EP 936218	A1	19990818	EP 1997-929510	19970703
	EP 936218	B1	20030402		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	AT 236133	E	20030415	AT 1997-929510	19970703
	KR 2000022398	A	20000425	KR 1998-710829	19981230
	US 6387938	B1	20020514	US 2000-614877	20000712
PRAI	JP 1996-176711	A	19960705		
	WO 1997-JP2308	W	19970703		
	US 1998-214274	B2	19981231		
	JP 2000-35283	A	20000214		

OS MARPAT 128:102090
GI



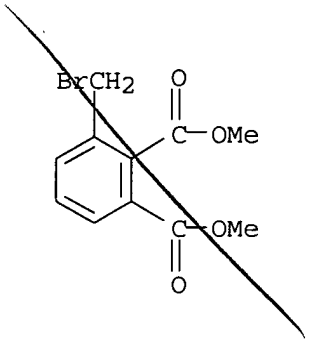
I

AB Novel benzimidazole derivs. represented by general formula [I; wherein R2 = cyano, hydroxymethyl, 2-(2-imidazolyl)ethenyl, Ph substituted by one or

two CO2R3 groups, CO2R3 or CONR4R5; wherein R3 = H, C1-4 linear or branched alkyl; R4, R5 = H, C1-2 alkyl, CH2CO2R6, CH(CH2Ph)CO2R6; when one of R4 and R5 = CH2CO2R6 or CH(CH2Ph)CO2R6, the other = H; wherein R6 = C1-4 linear or branched alkyl; A = a group selected from the group consisting of CO, CH(OR8), CH2O, CH(NHR9)CH2, CH:CH, and CH2CH2; wherein R8 = H, acetyl; R9 = H, acetyl, PhSO2, benzoyl optionally substituted by a MeO group; W = CH2 or a single bond; Q = Ph optionally substituted by a hydroxyl group; n = 0 to 2; R7 = H, OH, halo, C1-4 linear or branched alkyl] are prepared Also claimed are a process for producing I and drugs containing as the active ingredient at least one of I, in particular, preventives and/or remedies for diseases exhibiting acidophilia (eosinophilia or acidocytosis), bronchial asthma and allergic diseases. Thus, CO2(g) was blown into a mixture of 4-acetyl-2-(2-phenylethyl)benzimidazole (preparation given), K2CO3, 18-crown-ether, and DMSO under stirring at room temperature for 6 h to give, after workup, 3-[2-(2-phenylethyl)benzimidazol-4-yl]-3-oxopropanoic acid (II). II in vivo inhibited the increase of eosinophil counts in mice injected i.p. with pig ascaris extract by 67 and 78% at 3 and 30 mg/kg/day for 10 days, resp. Pharmaceutical formulations, e.g. capsules containing Et 3-[2-(2-phenylethyl)benzimidazol-4-yl]-3-hydroxypropanoate, were prepared

IT **24129-04-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel benzimidazole derivs. for treatment of acidophilia, bronchial asthma, and allergic disease)

RN 24129-04-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 52 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:65811 CAPLUS
DN 128:136515
TI Bone resorption inhibitors
IN Aibe, Kazuhiko; Takebayashi, Yukihiro; Ishii, Yasutaka; Noshiro, Osamu; Noda, Ichio; Igarashi, Susumu
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9801133	A1	19980115	WO 1997-JP2357	19970708

W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

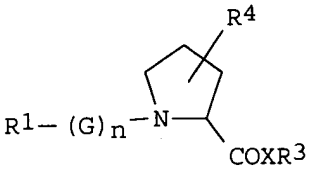
10803578

RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

	AU 9733596	A1	19980202	AU 1997-33596	19970708
PRAI	JP 1996-177955	A	19960708		
	WO 1997-JP2357	W	19970708		

OS MARPAT 128:136515

GI



I

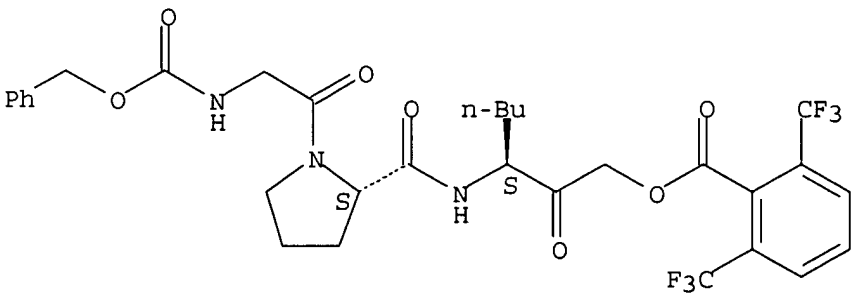
AB Drugs, in particular, bone resorption inhibitors containing as the active ingredient compds. having selective cathepsin K inhibitory effects, among all, proline derivs. represented by general formula (I) or pharmaceutically acceptable salts thereof, wherein each symbol has the meaning as specified below: X: a moiety (except for the C-terminal carbonyl group) of an amino acid residue with its side chain optionally protected; R1: an amino-protective group; G: a glycine residue; n: 0 or 1; R3: a group inhibiting the activity of the SH group of cysteine protease; and R4: hydrogen, hydroxy or Ph.

IT **202281-22-9P 202281-46-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(bone resorption inhibitors)

RN 202281-22-9 CAPLUS

CN L-Prolinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(1S)-1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 202281-46-7 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]amino]carbonyl]-, phenylmethyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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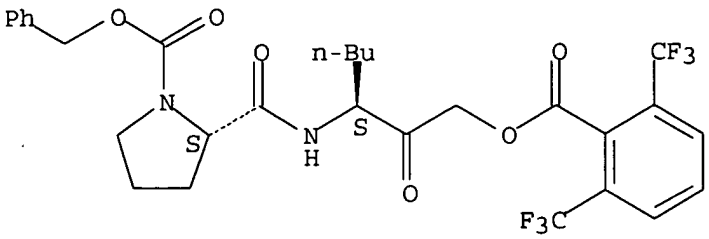


RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 53 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:717935 CAPLUS
DN 128:1461
TI Substrates and inhibitors of proteolytic enzymes
IN Quibell, Martin; Johnson, Tony; Hart, Terance
PA Peptide Therapeutics Ltd., UK; Quibell, Martin; Johnson, Tony; Hart, Terance
SO PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9740065	A2	19971030	WO 1997-GB1157	19970424
	WO 9740065	A3	19971204		
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2252508	AA	19971030	CA 1997-2252508	19970424
	AU 9726449	A1	19971112	AU 1997-26449	19970424
	AU 706855	B2	19990624		
	CA 2252408	AA	19971113	CA 1997-2252408	19970424
	EP 906333	A2	19990407	EP 1997-918252	19970424
	EP 906333	B1	20010725		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2001501170	T2	20010130	JP 1997-537864	19970424
	AT 203545	E	20010815	AT 1997-918252	19970424
	ES 2162277	T3	20011216	ES 1997-918252	19970424
	US 6528275	B1	20030304	US 1999-171680	19991103
	US 2003092067	A1	20030515	US 2002-259420	20020930
PRAI	GB 1996-8457	A	19960424		
	GB 1996-16115	A	19960731		
	GB 1996-24584	A	19961127		
	WO 1997-GB1157	W	19970424		
	US 1999-171680	A3	19991103		

AB The present invention relates to the field of compds. which are substrates or inhibitors of proteolytic enzymes and to apparatus and methods for identifying substrates or inhibitors for proteolytic enzymes. We have devised a combinatorial method for the rapid identification of binding motifs which will greatly expedite the synthesis of inhibitors of a variety of proteolytic enzymes such as aspartyl proteases, serine

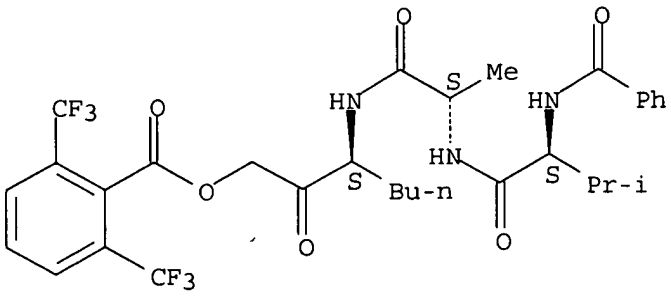
proteases, metallo proteases and cysteinyl proteases. Some inhibitors have the formula A-B-C-D-nE-F, in which A represents a fluorescor internally quenched by F; while B, C, D, and E represent groups such that the scissile bond between any two of these groups is a suitable bond; n is an integer 1, 2, 3, or 4; and F a quencher capable of internally quenching the fluorescor A.

IT **187991-44-2P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(substrates and inhibitors of proteolytic enzymes)

RN 187991-44-2 CAPLUS

CN L-Alaninamide, N-benzoyl-L-valyl-N-[(1S)-1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 54 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:381417 CAPLUS

DN 127:95064

TI A re-investigation of the reaction of hemimellitic acid with sulfur tetrafluoride. A simple preparation of 2,6-bis(trifluoromethyl)benzoic acid

AU Dmowski, Wojciech; Wiszniewski, Wojciech

CS Inst. Organic Chem., Polish Academy Sci., Warsaw, 01-224, Pol.

SO Journal of Fluorine Chemistry (1997), 82(2), 163-165
CODEN: JFLCAR; ISSN: 0022-1139

PB Elsevier

DT Journal

LA English

OS CASREACT 127:95064

AB The reaction of hemimellitic acid with SF4/HF gave a 1:3.5:13 mixture of 1,2,3-tris(trifluoromethyl)benzene, 1,1,3,3-tetrafluoro-4-trifluoromethyl-1,3-dihydroisobenzofuran and 2,6-bis(trifluoromethyl)benzoyl fluoride. Treatment of the crude reaction mixture with aqueous KOH, followed by acidification of the water phase, gave a good yield of pure 2,6-bis(trifluoromethyl)benzoic acid.

IT **24821-22-5P**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reductive fluorination of hemimellitic acid and preparation of bis(trifluoromethyl)benzoic acid)

RN 24821-22-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

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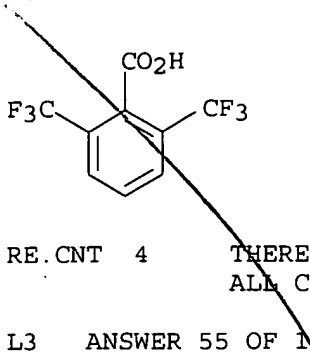


RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 55 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:220603 CAPLUS
DN 126:212446
TI Tripeptide methyl ketone cysteine protease inhibitors for use in treatment of Ige mediated allergic diseases
IN Johnson, Tony; Hart, Terrance; Laing, Peter; Shakib, Farouk; Quibell, Martin
PA Peptide Therapeutics Limited, UK; Johnson, Tony; Hart, Terrance; Laing, Peter; Shakib, Farouk; Quibell, Martin
SO PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

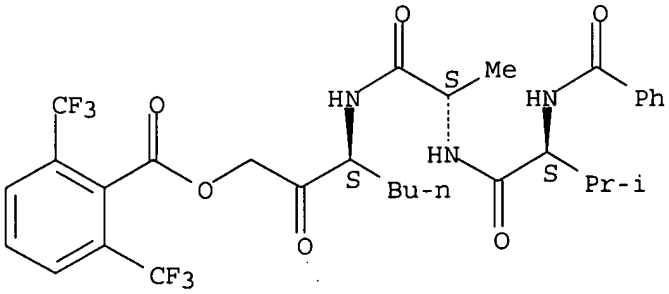
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9704004	A1	19970206	WO 1996-GB1707	19960717
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
	CA 2227198	AA	19970206	CA 1996-2227198	19960717
	AU 9665242	A1	19970218	AU 1996-65242	19960717
	AU 716716	B2	20000302		
	EP 839155	A1	19980506	EP 1996-924976	19960717
	EP 839155	B1	20041013		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 11509543	T2	19990824	JP 1996-506421	19960717
	AT 279433	E	20041015	AT 1996-924976	19960717
	US 6034066	A	20000307	US 1998-45	19980226
PRAI	GB 1995-14616	A	19950717		
	GB 1995-22221	A	19951031		
	WO 1996-GB1707	W	19960717		

OS MARPAT 126:212446
AB Tripeptide compds. were prepd for use in the treatment of allergic diseases, including juvenile asthma and eczema, via inhibition of the cysteine protease activity of Dermatophagoides pteronyssinus (Der p I), a major allergen of house dust mite. Compds. claimed included R1-CONH-XR2-CONH-YR3-CONH-ZR4-W [X, Y, Z = N, CH; R1 = nitrogen blocking group; R2, R3, R4 = side-chains on X, Y, Z; W = group that reacts irreversibly with active cysteine thiol of Der p I; R1 = hydrophobic Ph, 2-naphthyl, 9-anthracyl, heteroaryl optionally connected to heteroatom to carbonyl group, etc.; XR2 = Ala, Leu, Nle, Val, etc; YR3 = Lys, Gln, Met(O), Ala; ZR4 = Ala, Leu, Nle, Val, Ile, etc.; W = E-CH2CHO, E-CH2CH:CH2, E-CH2CH:CHCHO, R-CO2NCHO, Y-CH:CH2; E = aryloxy, arylthio, heteroaryl, halo, R-SO3, R2P(O)O, RCO2; R = alkyl, aryl; Y = ester, sulfone, carboxylate, amide, etc. groups]. E64, L-trans-epoxysuccinyl-leucylamido(4-guanidino)butane, is excluded from the claimed compds.

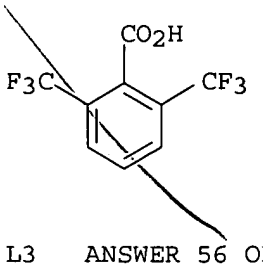
Thus, Bz-Val-Ala-Nle-OH underwent successive treatment with iso-Bu chloroformate/N-methylmorpholine, CH2N2, and HBr/HOAc to give Bz-Val-Ala-Nle-CH2Br which reacted with 2,6-Cl2C6H3CO2OH to give Bz-Val-Ala-Nle-CH2O2CC6H3Cl2-2,6 (I). In Der p I enzyme inhibiting assay, I had a Kobs/[I] of 6.8 x 107 M-1 s-1.

IT **187991-44-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tripeptide Me ketones with allergen inhibiting activity)
RN 187991-44-2 CAPLUS
CN L-Alaninamide, N-benzoyl-L-valyl-N-[(1S)-1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in preparation of tripeptide Me ketones with allergen inhibiting activity)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 56 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:206852 CAPLUS
DN 126:274659
TI Use of inhibitors to identify essential cysteine proteinases of Trichomonas vaginalis
AU Irvine, Joseph W.; North, Michael J.; Coombs, Graham H.
CS Infection and Immunity, Institute of Biological and Life Sciences, Joseph Black Building, University of Glasgow, Glasgow, G12 8QQ, UK
SO FEMS Microbiology Letters (1997), 149(1), 45-50
CODEN: FMLED7; ISSN: 0378-1097
PB Elsevier
DT Journal
LA English
AB Designing cysteine proteinase inhibitors as antitrichomonal drugs requires knowledge of which cysteine proteinases are essential to the parasite. To obtain such information, the effects of a number of cysteine proteinase inhibitors on trichomonad growth in vitro and proteinase activity were

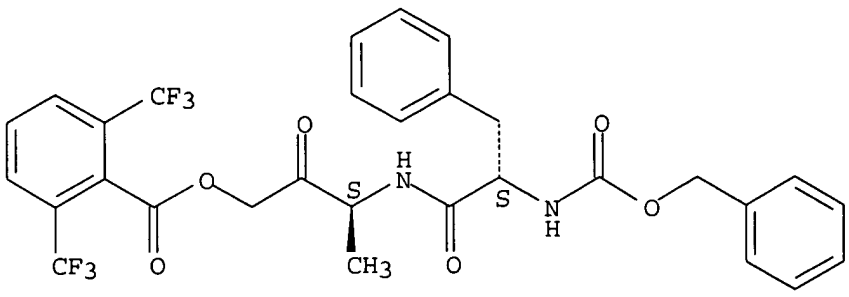
investigated. The broad specificity inhibitor trans-epoxysuccinyl-L-leucylamido-(4-guanidino)butane (known as E-64) had little effect on growth of Trichomonas vaginalis (27% inhibition at 280 μM, none at 28 μM) even though the addition of 2.8 μM E-64 to growth medium resulted in inhibition of all but two (apparent mol. masses: 35 k and 49 k) of the parasite's proteinases detected by gelatin SDS-PAGE. This shows that many of the parasite's cysteine proteinases are not essential for growth in axenic culture. In contrast, a peptidyl acyloxymethyl ketone, N-benzoyloxycarbonyl-Phe-Ala-CH2OCO-(2,6,-(CF3)2)Ph, at 16 μM killed T. vaginalis and severely inhibited growth of Tritrichomonas foetus. Exposure of Trichomonas vaginalis to 16 μM of this compound for 1 h resulted in both the 35 kDa and 49 kDa proteinases being inhibited, whereas some other proteinases were unaffected. Similar distinctions between the inhibitor sensitivity of the parasite's cysteine proteinases were apparent when a biotinylated peptidyl diazomethyl ketone was used to detect active proteinases. These data suggest that the growth inhibitory effects of the peptidyl acyloxymethyl ketone are through inhibition of cysteine proteinases that are not affected when the parasites are grown in the presence of E-64. At least one of these enzymes, which include the 35 kDa and 49 kDa cysteine proteinases, must be essential and so a suitable target for chemotherapeutic attack.

IT **115186-03-3**
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); PROC (Process); USES (Uses)
(use of inhibitors to identify essential cysteine proteinases of Trichomonas vaginalis)

RN 115186-03-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 57 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:145222 CAPLUS

DN 126:144557

TI Preparation of peptidyl ketones as calpain inhibitors for the treatment of neurodegenerative diseases

IN Dolle, Roland E.; Graybill, Todd L.; Osifo, Irennegbe K.; Harris, Alex L.; Miller, Matthew S.

PA Sanofi Winthrop, Inc., USA

SO PCT Int. Appl., 56 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	WO 9641638	A1	19961227	WO 1995-US7463	19950613
	W: AU, CA, HU, JP, MX				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2224721	AA	19961227	CA 1995-2224721	19950613
	AU 9527043	A1	19970109	AU 1995-27043	19950613
	EP 840614	A1	19980513	EP 1995-922312	19950613
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
PRAI	WO 1995-US7463	A	19950613		

OS MARPAT 126:144557

AB Novel amino acid analogs Z-A3-A2-A1-Q [Z = H, protecting group; A3, A2 = independently optionally protected Val, Leu, Ala, Ile, Phe, Tyr, Gly, D- or L-2-arylglycine, bond; A1 = optionally protected Val, Leu, Ile, Ala, Phe, Tyr, 2-phenylglycine, 2-phenethylglycine, 2-arylglycine; Q = H, CH2O2C-L, CH2O-L, CH2S-L, CH2X, NHNHCOCH2O2C-L, NHNHCOCH2O-L, NHNHCOCH2S-L; L = (un)substituted aryl or (un)substituted heteroaryl; X = Cl, Br, F] and pharmaceutically acceptable salt thereof are provided as calpain inhibitors. Thus, condensation of Cbz-Leu-Phe-OH (Cbz = PhCh2O2C) with iso-Bu chloroformate and N-methylmorpholine in THF, followed by reaction with etherial CH2N2 and treatment with HBr in AcOH gave protected bromomethyl ketone Cbz-Leu-Phe-CH2Br (I) in 86% yield. Substitution of I with 2,6-F2C6H3CO2H gave 70% aryloxymethyl ketone Cbz-Leu-Phe-CH2O2CC6H3F2-2,6, which was deprotected by catalytic hydrogenolysis and coupled with Cbz-D-Ala-OH to give peptidyl aryloxymethyl ketone Cbz-D-Ala-Leu-Phe-CH2O2CC6H3F2-2,6 (II). I and II inhibited human calpain I with IC50 = 9.1 μM and 0.046 μM, resp.

IT **115186-03-3P 186692-98-8P**

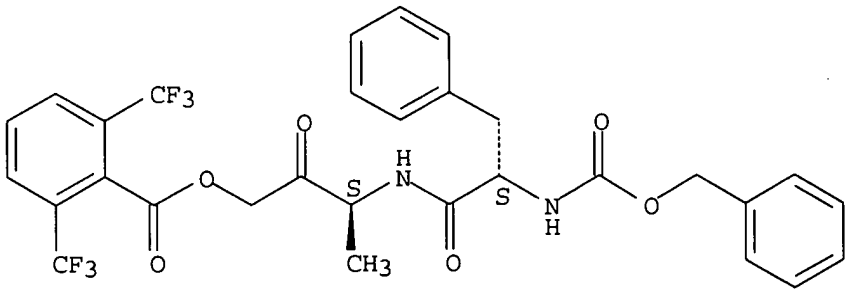
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of peptidyl ketones as calpain inhibitors for the treatment of neurodegenerative diseases)

RN 115186-03-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

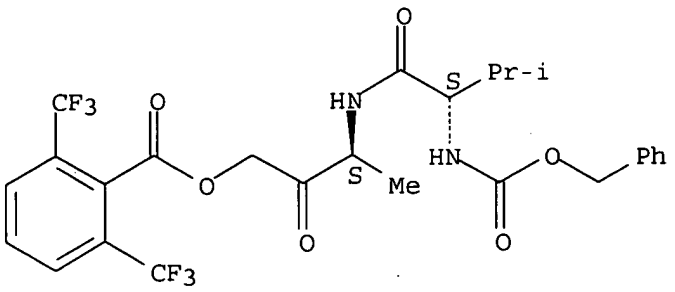
Absolute stereochemistry.



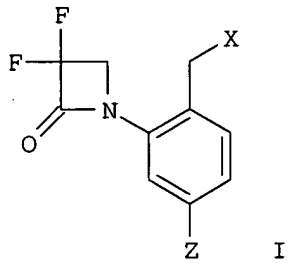
RN 186692-98-8 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 3-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-2-oxobutyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 58 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:75738 CAPLUS
DN 126:199403
TI Synthesis and inhibition of human leukocyte elastase by functionalized N-Aryl 2-azetidinones: effect of different substituents on the aromatic ring
AU Joyeau, R.; Felk, A.; Guilaume, S.; Wakselman, M.; Vergely, I.; Doucet, C.; Boggetto, N.; Reboud-Ravaux, M.
CS SIRCOB, Batiment Lavoisier, Universite de Versailles-St Quentin en Y, Versailles, 78000, Fr.
SO Journal of Pharmacy and Pharmacology (1996), 48(12), 1218-1230
CODEN: JPPMAB; ISSN: 0022-3573
PB Royal Pharmaceutical Society of Great Britain
DT Journal
LA English
GI

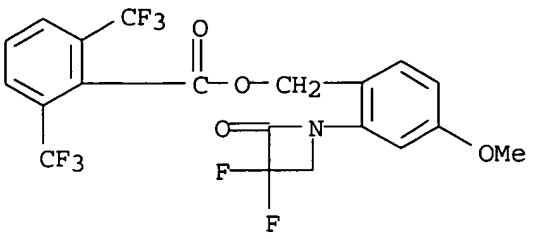


I

AB N-aryl-3,3-difluoro-2-azetidinones I (X = H, Cl, F, OAc, etc.; Z = H, OMe, etc.) which feature a latent electrophilic methylene quinoniminium function were synthesized and evaluated as inhibitors of human leukocyte elastase. To promote hydrophobic interactions with the enzyme, to increase the rates of β-lactam ring opening and of benzylic group departure, or to induce hydrosoly., these compds. incorporate on their aromatic ring either an alkyl moiety, a methoxy substituent or a carboxylic group. Some of these β-lactams proved to be good inactivators of human leukocyte elastase.

IT **187731-97-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (aryl)difluoroazetidinones as leukocyte elastase inhibitors)
RN 187731-97-1 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, [2-(3,3-difluoro-2-oxo-1-azetidinyl)-4-methoxyphenyl]methyl ester (9CI) (CA INDEX NAME)

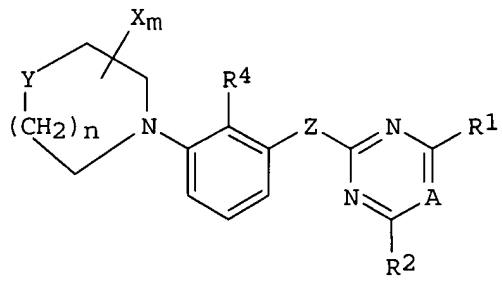
10803578



L3 ANSWER 59 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:53965 CAPLUS
DN 126:74874
TI Preparation of substituted benzoic acid derivatives as herbicides
IN Ueda, Akiyoshi; Miyazawa, Yasuyuki; Sato, Daisuke; Koguchi, Masami; Matsumoto, Isoko; Kawana, Takashi
PA Nippon Soda Co., Ltd., Japan; Ueda, Akiyoshi; Miyazawa, Yasuyuki; Sato, Daisuke; Koguchi, Masami; Matsumoto, Isoko; Kawana, Takashi
SO PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9636613	A1	19961121	WO 1996-JP1262	19960514
W: BR, CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
PRAI JP 1995-145503	A	19950519		

OS MARPAT 126:74874
GI



I

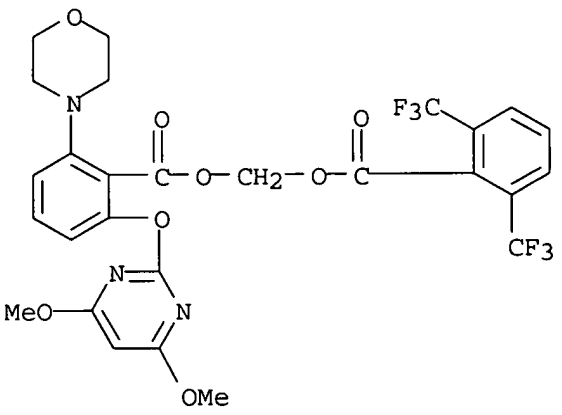
AB The title compds. (I; A = R3 substituted N or C; Z = O, S, etc.; R1, R2 = H, C1-6 alkyl or alkoxy, cyano, etc.; R3 = H, C1-6 alkyl, halo, NO2, etc.; R4 = CO2R7, CHO, COR8, CHR8OR9, CR8:NOR10, etc.; X = C1-6 alkyl, C3-7 cycloalkyl, etc.; m = 0-4; Y = O, S, CO, CS, R5CR5', C:NR6, NR6; R5, R5' = H, C1-6 alkyl, etc.; R6 = H, C1-6 alkyl or haloalkyl, etc.; R7 = H, C1-6 alkyl or haloalkyl, etc.; R8 = C1-6 alkyl or haloalkyl, etc.; R9, R10 = H, C1-6 alkyl or haloalkyl, C3-7 cycloalkyl, etc.; n = 0-3) are prepared I exhibiting excellent herbicidal activity are useful as herbicides. Thus, 2-hydroxy-6-morpholinobenznitrile was reacted with 4,6-dimethoxy-2-methanesulfonylpyrimidine in the presence of K2CO3 to give I (R1 = R2 = OMe, A = CR3, R3 = Xm = H, R4 = cyano, Y = Z = O, n = 1). Herbicides containing I (R1 = R2 = OMe, A = CR3, R3 = Xm = H, R4 = CO2H, Y = Z = O, n = 1) at 63 g/ha postemergence showed 100% herbicidal effect for Xanthium

pensylvanicum, Setaria faberii, Abutilon theophrasti, and Amaranthus lividus.

IT **185398-70-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted benzoic acid derivs. as herbicides)

RN 185398-70-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, [[2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-6-(4-morpholinyl)benzoyl]oxy]methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 60 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:38492 CAPLUS

DN 126:118191

TI Total synthesis of cyclothialidine

AU Goetschi, Erwin; Jenny, Christian Johannes; Reindl, Peter; Ricklin, Fabienne

CS Pharma Division, Hoffmann-La Roche Ltd., Basel, CH-4002, Switz.

SO Helvetica Chimica Acta (1996), 79(8), 2219-2234
CODEN: HCACAV; ISSN: 0018-019X

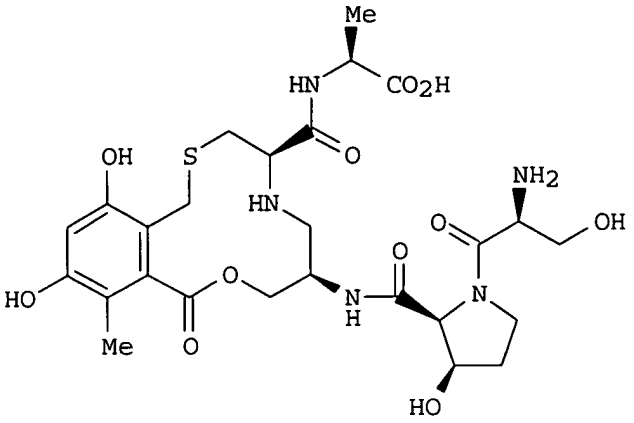
PB Verlag Helvetica Chimica Acta

DT Journal

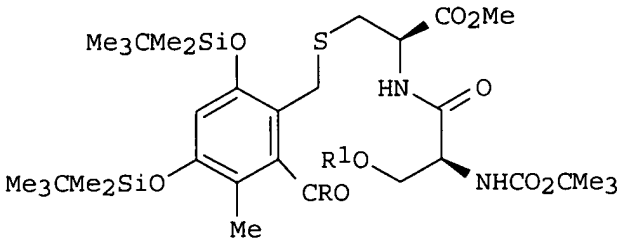
LA English

OS CASREACT 126:118191

GI



I



II

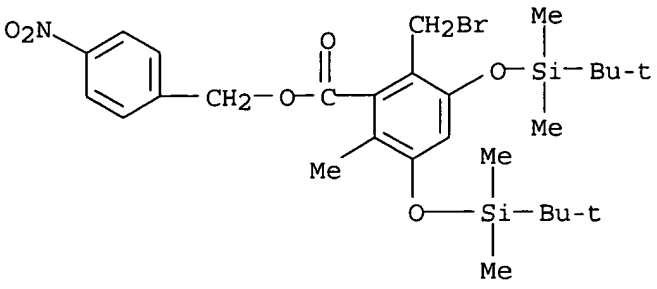
AB A total synthesis of cyclothialidine I, a DNA gyrase inhibitor isolated from Streptomyces filipinensis, is described. The synthetic concept was tested by preparing a lactone containing the bicyclic core entity of I. Key features of the synthesis of I are preparation of 3,5-dihydroxy-2,6-dimethylbenzoate from 3,5-dihydroxybenzoate by 2 consecutive Mannich aminomethylation/hydrogenation sequences, benzylic N-bromosuccinimide bromination of an ester derivative thereof and its subsequent coupling with Boc-Ser-Cys-OMe, cyclization of the ω-hydroxy acid II (R = OH, R1 = H) to the 12-membered lactone II (RR1 = bond) using preferably Mitsunobu conditions, and completion of the peptidic side chains of I using Boc strategy. Optically pure cis-N-(tert-butoxycarbonyl)-3-hydroxy-L-proline was obtained by resolution of the racemate via an efficient reaction sequence containing a lipase-catalyzed enantiospecific acetate hydrolysis. The structure of natural I was confirmed by comparison with the synthetic material. The synthetic route described provides also easy access to analogs of I.

IT **147214-70-8P 186132-87-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of cyclothialidine)

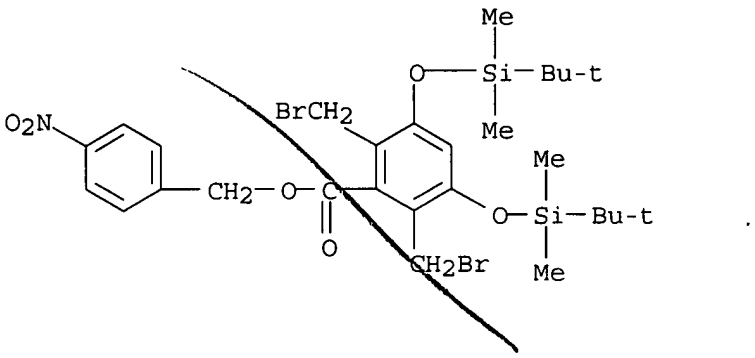
RN 147214-70-8 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

10803578



RN 186132-87-6 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 61 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:718301 CAPLUS
DN 126:19327
TI Preparation of peptide compounds as cysteine protease inhibitors
IN Fukuda, Tsunehiko; Fujisawa, Yukio; Watanabe, Hiroyuki
PA Takeda Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9630395	A2	19961003	WO 1996-JP840	19960329
	WO 9630395	A3	19961227		
	W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	JP 09165360	A2	19970624	JP 1996-73861	19960328
	CA 2215211	AA	19961003	CA 1996-2215211	19960329
	AU 9651221	A1	19961016	AU 1996-51221	19960329
	EP 820464	A2	19980128	EP 1996-907705	19960329
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	US 6162828	A	20001219	US 1996-648145	19960520
PRAI	JP 1995-75593	A	19950331		
	JP 1995-75594	A	19950331		

JP 1995-265723 A 19951013
WO 1996-JP840 W 19960329

OS MARPAT 126:19327

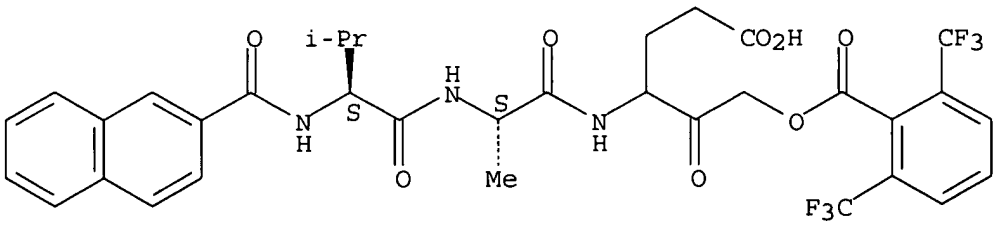
AB Peptide derivs. R1-R2-R3-R4-NHA(Z)(CH2)nCO2H [I; R1 = H, acyl; R2 - R4 = a bond, an amino acid residue, a group of the formula Y-R5, in which R5 is a group resulting from imino group removal from an amino acid residue; Y = O, S, NR6, in which R6 = H or lower alkyl; A = CH, N; Z = H, an acyl group, an optionally substituted hydrocarbon group; n = 1 or 2; provided that when n = 1, then A = CH and Y = S or NR6, and, at least one of R2, R3 and R4 = the formula Y-R5, provided that when further all Y = NR6, at least one of the amino acid residues is not bound to an hydrogen atom at the α-carbon thereof but substituted via carbon; provided that when n = 2 and Z = an aldehyde group, then R1 = an acyl group having 6 or more carbon atoms; provided that when n = 2 and A is CH, then at least one of R2, R3 and R4 is the formula Y-R5] or esters or salts thereof are prepared A pharmaceutical composition containing I is useful for inhibiting interleukin-1β converting enzyme or cysteine protease and for treating or preventing rheumatic arthritis or septic shock. Thus, Fmoc-Val-Aib-OH (Aib = α-aminoisobutyric acid residue) was condensed with H2NCH[CH(OMe)2]CH2CO2CMe3 using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBt in DMF at 0° for 1 h and at 28° for 14 h to give Fmoc-Val-Aib-NHCH[CH(OMe)2]CH2CO2CMe3, which was treated with aqueous CF3CO2H at 28° for 4 h to give Fmoc-Val-Aib-NHCH(CHO)CH2CO2H. The latter compound in vitro showed IC50 of 1.9 + 10-8 M against recombinant interleukin-1β converting enzyme.

IT **183438-75-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptide compds. as inhibitors of cysteine protease and interleukin-1β converting enzyme for treating septic shock and rheumatic arthritis)

RN 183438-75-7 CAPLUS

CN L-Alaninamide, N-(2-naphthalenylcarbonyl)-L-valyl-N-[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(2-carboxyethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

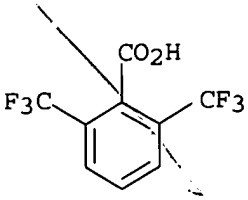


IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptide compds. as inhibitors of cysteine protease and interleukin-1β converting enzyme for treating septic shock and rheumatic arthritis)

RN 24821-22-5 CAPLUS

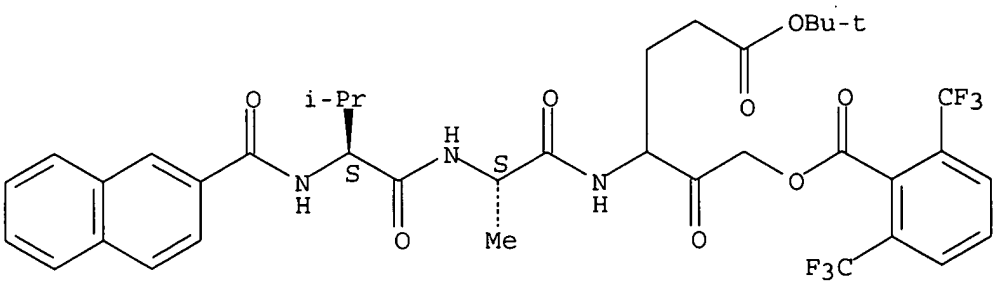
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

10803578



IT **183439-95-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide compds. as inhibitors of cysteine protease and interleukin-1β converting enzyme for treating septic shock and rheumatic arthritis)
RN 183439-95-4 CAPLUS
CN L-Alaninamide, N-(2-naphthalenylcarbonyl)-L-valyl-N-[1-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]acetyl]-4-(1,1-dimethylethoxy)-4-oxobutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

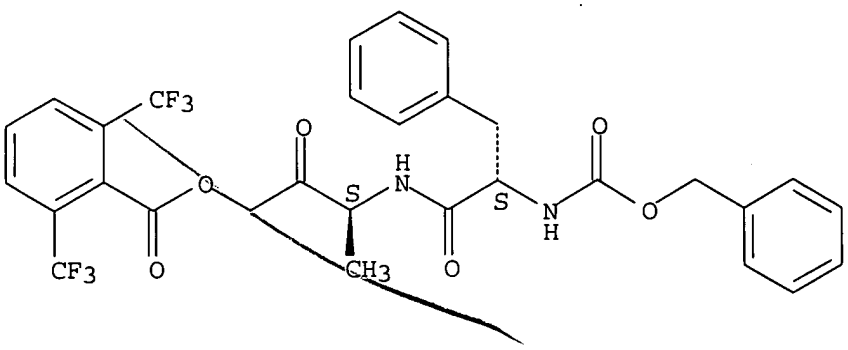


L3 ANSWER 62 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:583102 CAPLUS
DN 125:292311
TI Cysteine protease inhibitors block schistosome hemoglobin degradation in vitro and decrease worm burden and egg production in vivo
AU Wasilewski, Margaret M.; Lim, K. C.; Phillips, Jennifer; McKerrow, James H.
CS Department of Medicine, University of California, San Francisco, San Francisco, CA, USA
SO Molecular and Biochemical Parasitology (1996), 81(2), 179-189
CODEN: MBIPDP; ISSN: 0166-6851
PB Elsevier
DT Journal
LA English
AB Schistosome parasites utilize Hb as a major protein source for their metabolism Degradation of Hb has been hypothesized to be mediated by both cysteine and aspartyl proteases secreted into the lumen of the parasite intestine. We now show that two distinct types of irreversible cysteine protease-specific inhibitors both arrest schistosome Hb degradation in vitro. Arrest of Hb degradation is followed by death of developing schistosomula 1 wk later. Schistosome infected mice treated by a dose of 2 mg inhibitor per day for 1 wk early in infection, and 2 wk at the time of egg production, showed a significant reduction in worm burden, hepatomegaly, and the number of eggs produced per female worm. Histopathol. showed a minimal immune response to those eggs which were produced, consistent with a delay in egg production relative to untreated infections. By tagging the inhibitor with biotin, specific cysteine protease targets were identified in exts. of schistosome worms.

10803578

IT **115186-03-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cysteine protease inhibitors block schistosome Hb degradation in vitro and decrease worm burden and egg production in vivo)
RN 115186-03-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

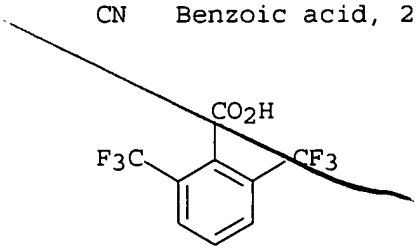
Absolute stereochemistry.



L3 ANSWER 63 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:569367 CAPLUS
DN 125:195049
TI Preparation of cycloalkanols by catalytic hydration of cycloalkenes
IN Moryasu, Masataka; Setoyama, Tooru; Takewaki, Takahiko; Yamaguchi, Takahiro; Fujita, Naoko; Maki, Takao
PA Mitsubishi Chemical Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 08176040	A2	19960709	JP 1994-315020	19941219
PRAI JP 1994-315020		19941219		

OS CASREACT 125:195049
AB Cycloalkanols are prepared in high yield by hydration of cycloalkenes in the presence of solid catalysts and fluorobenzoic acids. A mixture of cyclohexene, H2O, H gallosilicate (preparation given), and C6F5CO2H (I) was autoclaved at 120° for 30 min yo give 16.9% cyclohexanol, vs. 13.1% for a control using PhCO2H instead of I.
IT **24821-22-5**, 2,6-Di(trifluoromethyl)benzoic acid
RL: CAT (Catalyst use); USES (Uses)
(preparation of cycloalkanols by hydratio of cycloalkenes using solid acids and fluorobenzoic acids)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



10803578

L3 ANSWER 64 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:323963 CAPLUS
DN 125:58504
TI 2-Saccharinylmethyl arylcarboxylates useful as proteolytic enzyme inhibitors and compositions and method of use thereof
IN Dunlap, Richard P.; Boaz, Neil W.; Mura, Albert J.; Kumar, Virendra; Subramanyam, Chakrapani; Desai, Ranjit C.; Hlasta, Dennis J.; Saindane, Manohar T.; Bell, Malcolm R.; et al.
PA Sterling Winthrop Inc., USA
SO U.S., 52 pp., Cont.-in-part of U.S. 5,306,818.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 7

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5512589	A	19960430	US 1993-116416	19930903
	US 5128339	A	19920707	US 1991-782016	19911024
	IL 114773	A1	19961205	IL 1991-114773	19911031
	US 5250696	A	19931005	US 1992-860340	19920330
	NO 9202976	A	19920504	NO 1992-2976	19920728
	NO 301116	B1	19970915		
	US 5306818	A	19940426	US 1992-965593	19921023
	US 5380737	A	19950110	US 1993-113508	19930827
	HU 70756	A2	19951030	HU 1994-569	19940225
	HU 70764	A2	19951030	HU 1994-580	19940225
	US 5464852	A	19951107	US 1994-289113	19940811
	FI 9404968	A	19941021	FI 1994-4968	19941021
	US 5578623	A	19961126	US 1995-445240	19950519
	US 5597841	A	19970128	US 1995-445118	19950519
	FI 9600490	A	19960202	FI 1996-490	19960202
	FI 103115	B1	19990430		
	US 5773456	A	19980630	US 1996-719216	19960925
PRAI	US 1990-608068	B2	19901101		
	US 1991-782016	A3	19911024		
	US 1992-860340	A2	19920330		
	US 1992-965593	A2	19921023		
	US 1989-347125	B2	19890504		
	US 1989-347126	B2	19890504		
	US 1990-514920	A	19900426		
	HU 1991-3430	A	19911031		
	IL 1991-99913	A3	19911031		
	FI 1991-5163	A	19911101		
	NO 1991-4288	A1	19911101		
	US 1991-793035	B1	19911115		
	US 1993-113508	A3	19930827		
	US 1993-116416	A3	19930903		
	US 1994-289113	A3	19940811		
	FI 1994-4968	A	19941021		
	US 1995-445240	A3	19950519		

OS MARPAT 125:58504
GI

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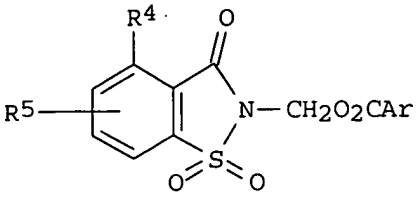


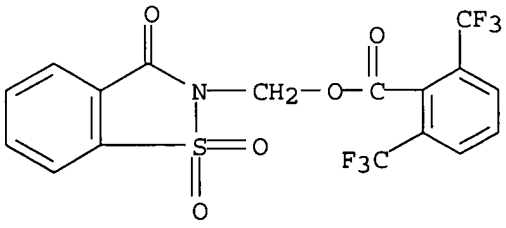
I

AB Title compds. I wherein: Ar is Ph, naphthyl or anthryl or such groups substituted by from one to three, the same or different, members of the group consisting of, e.g., lower alkyl, perfluoro lower alkyl, perchloro lower alkyl, lower alkoxy, halogen, nitro, cyano, carboxy; R4 = e.g., H, halo, lower alkyl; R5 = H or from one to two of the same or different substituents in any of the 5-, 6- or 7-positions selected from, e.g., halogen, cyano, nitro; with the proviso that, when R4 and R5 are independently either H or lower alkyl, then Ar cannot be either Ph, 2,4-dichlorophenyl or 4-nitrophenyl, have pharmaceutical utility as proteolytic enzyme inhibitors. Thus, e.g., esterification of 2,6-dichlorobenzoic acid with 2-chloromethyl-4,6-dimethoxysaccharin (preparation given as follows: 2,4-dimethoxy-N,N-diethylbenzamide → 2-aminosulfonyl-2,4-dimethoxy-N,N-diethylbenzamide → diethylammonium salt of 4,6-dimethoxysaccharin → 2-phenylthiomethyl-4,6-dimethoxysaccharin → 2-chloromethyl-4,6-dimethoxysaccharin) afforded 4,6-dimethoxy-2-saccharinylmethyl 2,6-dichlorobenzoate which exhibited inhibition of HLE (human leukocyte elastase) with Ki* (which is defined as the ratio of the koff/kon, the rate of reactivation of the enzyme to the rate of inactivation of the enzyme) = 0.08 nM.

IT **142426-83-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(2-saccharinylmethyl arylcarboxylates useful as proteolytic enzyme inhibitors)

RN 142426-83-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 65 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:230757 CAPLUS

DN 125:10520

TI Aromatic spirans. XXI. Syntheses of methyl substituted phthalaldehydic acids and their ethyl and methyl esters as synthones for syntheses of methylated 2,2'-spirobiindandiones

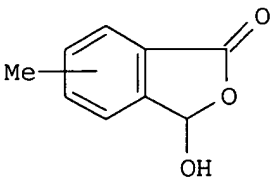
AU Neudeck, H. K.

CS Inst. Organische Chemie, Univ. Wien, Vienna, A-1090, Austria

SO Monatshefte fuer Chemie (1996), 127(2), 201-17

10803578

CODEN: MOCMB7; ISSN: 0026-9247
PB Springer
DT Journal
LA German
GI

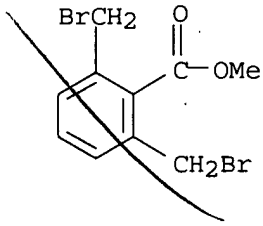


I

AB The preparation of 3-hydroxy(methyl)-1(3H)-isobenzofuranones I (i.e., phthalaldehydic acids) was described. I are intermediates for methylated 2,2'-spirobiindandiones (no data).

IT **56263-51-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (hydroxy)(methyl)isobenzofuranones)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 66 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:171795 CAPLUS
DN 124:232062
TI Preparation of amide group-containing cholecystokinin and gastrin receptor antagonists
IN Kalindjian, Sarkis Barret; Buck, Ildiko Maria; Dunstone, David John; Steel, Katherine Isobel Mary
PA James Black Foundation Ltd., UK
SO PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9530647	A1	19951116	WO 1995-GB997	19950502

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

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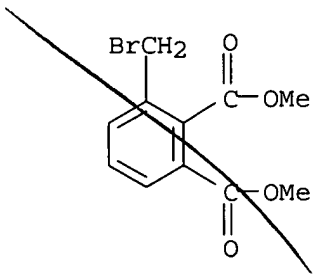
	AU 9523171	A1	19951129	AU 1995-23171	19950502
	GB 2303369	A1	19970219	GB 1996-23674	19950502
	GB 2303369	B2	19980527		
	ZA 9503739	A	19961111	ZA 1995-3739	19950509
	US 5939437	A	19990817	US 1996-737317	19961220
PRAI	GB 1994-9150	A	19940509		
	WO 1995-GB997	W	19950502		

OS MARPAT 124:232062
GI For diagram(s), see printed CA Issue.
AB The title compds. [I; Ar = (un)substituted monocyclic aromatic group; R1 = halogen, amino, nitro, cyano, sulfamoyl, sulfonyl, CF3, alkyl, alkylamino, dialkylamino, (un)substituted Ph, etc.; m = 0-4, provided that m is not more than 2 unless R1 is halogen; x + y = 0 or 1; R2, R4 = H, alkyl, etc.; R3 = H, (un)substituted C1-15 hydrocarbyl; R5 = H, C1-3 alkyl; U = (un)substituted aryl, (un)substituted heterocyclic, substituted heterocyclic, cycloalkyl; Z = (un)substituted heterocyclo, (un)substituted (phenylalkyl)amino or phenylamino], useful as cholecystokinin and gastrin receptor antagonists, are prepared Thus, [1S-(3,5-dicarboxyphenylaminocarbonyl)-2-phenylethylaminocarbonyl]-2-(1-adamantanemethylaminocarbonyl)benzene di-N-methyl-D-glucamine salt, prepared in 8 steps from 5-nitroisophthalic acid, demonstrated a CCKB receptor pKi of 7.1.
IT **24129-04-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amide group-containing cholecystokinin and gastrin receptor antagonists)
RN 24129-04-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

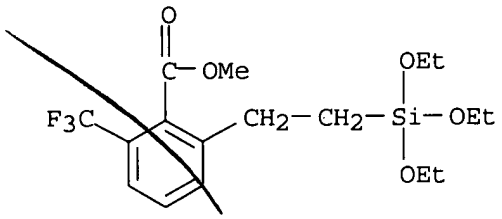


L3 ANSWER 67 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:98957 CAPLUS
DN 124:260516
TI Ruthenium-catalyzed addition of aromatic esters at the ortho C-H bonds to olefins
AU Sonoda, Motohiro; Kakiuchi, Fumitoshi; Kamatani, Asayuki; Chatani, Naoto; Murai, Shinji
CS Dep. Applied Chem., Osaka Univ., Suita, 565, Japan
SO Chemistry Letters (1996), (2), 109-10
CODEN: CMLTAG; ISSN: 0366-7022
PB Nippon Kagakkai
DT Journal
LA English
OS CASREACT 124:260516
AB A Ru complex, Ru(H)2(CO)(PPh3)3, can catalyze the addition of aromatic and heteroarom. esters at the ortho carbon-hydrogen bond to olefinic double bonds. While unsubstituted alkyl benzoate did not react, those substituted with CF3 or F underwent smooth catalytic addition A heteroarom.

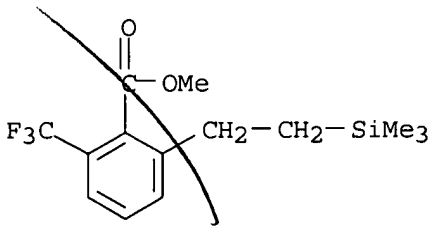
ester, 2-thiophenecarboxylic acid Et ester, and a benzo-δ-lactone, i.e., 1(3H)-isobenzofuranone and 1H-2-benzopyran-1-one were also treated under the same reaction conditions.

IT **175434-90-9P 175434-98-7P 175434-99-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective ruthenium-catalyzed addition of aromatic esters to alkenes)

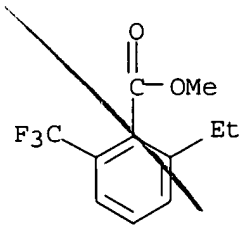
RN 175434-90-9 CAPLUS
CN Benzoic acid, 2-[2-(triethoxysilyl)ethyl]-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 175434-98-7 CAPLUS
CN Benzoic acid, 2-(trifluoromethyl)-6-[2-(trimethylsilyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 175434-99-8 CAPLUS
CN Benzoic acid, 2-ethyl-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 68 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:1003900 CAPLUS
DN 124:117626
TI Fluorinated phenylrhodopsin analogs. Binding selectivity, restricted rotation and 19F-NMR studies
AU Colmenares, Leticia U.; Liu, Robert S. H.
CS Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA
SO Tetrahedron (1996), 52(1), 109-18
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier
DT Journal
LA English

10803578

GI

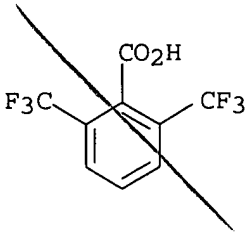
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Results from interactions of the 11-cis and 9-cis isomers of eleven fluorinated phenylretinal analogs I, II, III and IV, prepared from fluorinated benzaldehydes, with bovine opsin have been examined Five of these (2',6'-bis-CF3, 2',4',6'-tris-CF3, 2'-CF3-6'-F, 2'-CF3-7-Me and 2'-CF3,6'-F,8-F) formed pigments in moderate to high yields, thus allowing recording of their 19F-NMR spectra which revealed inhibited conformational equilibration when protein bound. Possible causes for binding selectivity and fluorine chemical shifts are discussed.

IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(binding selectivity, restricted rotation and 19F-NMR studies of fluorinated phenylrhodopsin analogs)

RN 24821-22-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 69 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:995314 CAPLUS

DN 124:146213

TI Preparation of mono- and bicyclic DNA gyrase inhibitors.

IN Geiwiz, Juergen; Goetschi, Erwin; Hebeisen, Paul; Link, Helmut; Luebbers, Thomas

PA F. Hoffmann-La Roche AG, Switz.

SO Eur. Pat. Appl., 92 pp.
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 675122	A2	19951004	EP 1995-103702	19950315
	EP 675122	A3	19971105		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CA 2144499	AA	19951001	CA 1995-2144499	19950313
	US 5589473	A	19961231	US 1995-407730	19950320
	ZA 9502380	A	19951220	ZA 1995-2380	19950323
	AU 9515070	A1	19951012	AU 1995-15070	19950324
	AU 694936	B2	19980806		
	HU 72491	A2	19960528	HU 1995-860	19950324
	IL 113123	A1	19991130	IL 1995-113123	19950324
	NO 9501210	A	19951002	NO 1995-1210	19950329
	FI 9501514	A	19951001	FI 1995-1514	19950330
	JP 07285953	A2	19951031	JP 1995-73217	19950330
	CN 1114648	A	19960110	CN 1995-104354	19950330
	BR 9501292	A	19960423	BR 1995-1292	19950330
	US 5594135	A	19970114	US 1995-541077	19951011

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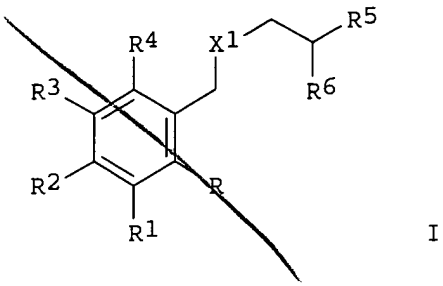
	US 5665746	A	19970909	US 1995-540678	19951011
	CN 1308071	A	20010815	CN 2000-135099	20001201
PRAI	EP 1994-104995	A	19940330		
	EP 1995-101595	A	19950207		
	US 1995-407730	A3	19950320		

OS MARPAT 124:146213

GI



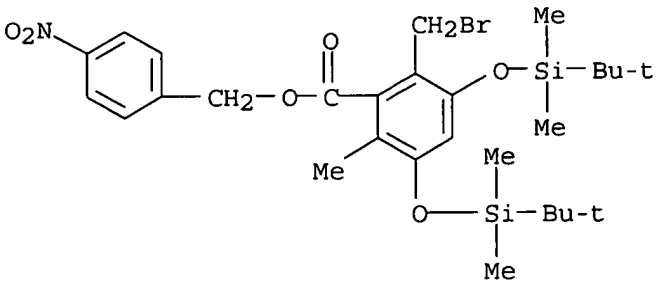
I

AB Title compds. [I; X1 = S, SO; R = cyano, (substituted) esterified carboxy, heterocyclyl; R1 = H, halo, alkyl, haloalkyl; R2 = H, OH, amino, alkylamino, dialkylamino, (substituted) alkoxy, OP; OP = easily hydrolyzable group; R3 = H, OH, alkyl, halo, OP; R4 = halo, OH, OP; R5 = H, cyano, (substituted) esterified carboxy, (substituted) amidated (thio)carboxy, (substituted) alkyl, alkenyl, heterocyclyl; R6 = NR7A, N:B, (substituted) heterocyclyl; R7 = H, alkyl; A = (substituted) iminoyl, thioacyl, (esterified) carboxy, amidated (thio)carboxy, heterocyclyl; B = (substituted) alkylidene; RR6 = CO2QX2NR7; X2 = (thio)carbonyl, heterocyclyl; Q = CHR8, CHR8W; R8 = H, (substituted) alkyl; W = (substituted) mono-, di-, tri-, tetra-, or pentamethylene; when W = monomethylene, then X2 ≠ (thio)carbonyl], were prepared Thus, (R)-N-[2-(2-aminocarbonyl-6-tert-butyldimethylsilyloxy-4-methoxy-3-methylbenzylsulfanyl)-1-(3-methyl-1,2,4-oxadiazol-5-yl)ethyl]acetamide (preparation given) in CH2Cl2 was treated with Cl3CCOCl and Et3N at 0° to room temperature to give (R)-N-[2-(2-cyano-6-hydroxy-4-methoxy-3-methylbenzylsulfanyl)-1-(3-methyl-1,2,4-oxadiazol-5-yl)ethyl]acetamide. A capsule formulation containing the latter are given. I showed IC50 = 1 to >64 μg/mL against Pseudomonas aeruginosa 799/61.

IT **147214-70-8P 173152-67-5P 173152-68-6P**
173152-72-2P 173152-73-3P 173152-74-4P
173152-75-5P 173152-76-6P 173152-77-7P
173152-81-3P 173152-90-4P 173152-93-7P
173153-35-0P 173153-79-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of mono- and bicyclic DNA gyrase inhibitors)

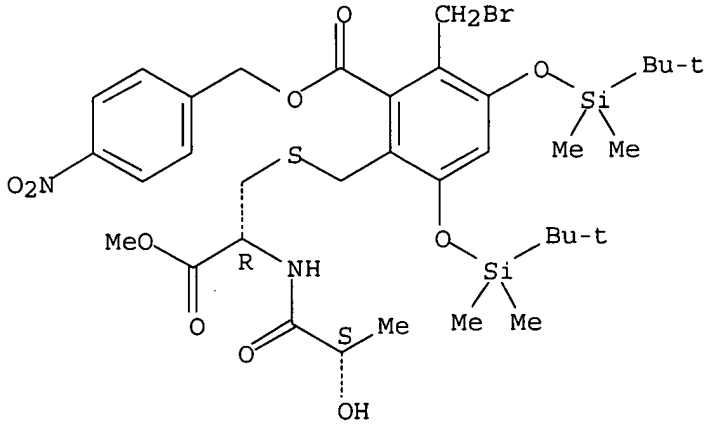
RN 147214-70-8 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



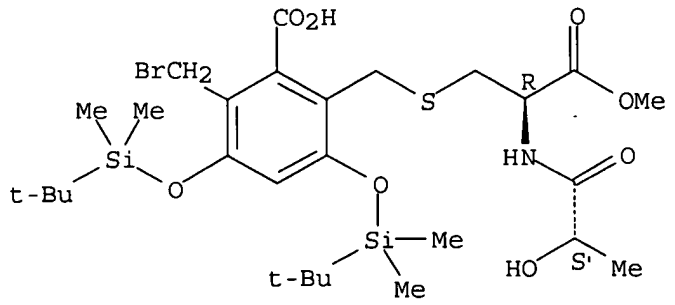
RN 173152-67-5 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[(2-hydroxy-1-oxopropyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-, (4-nitrophenyl)methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

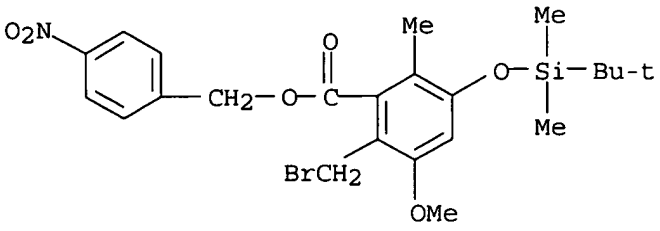


RN 173152-68-6 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[(2-hydroxy-1-oxopropyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

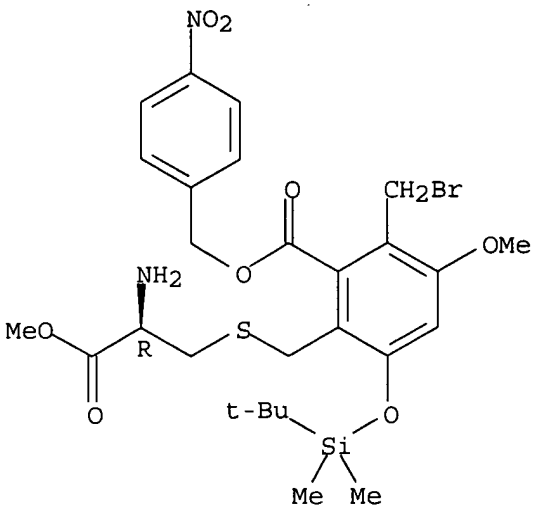


RN 173152-72-2 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methoxy-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



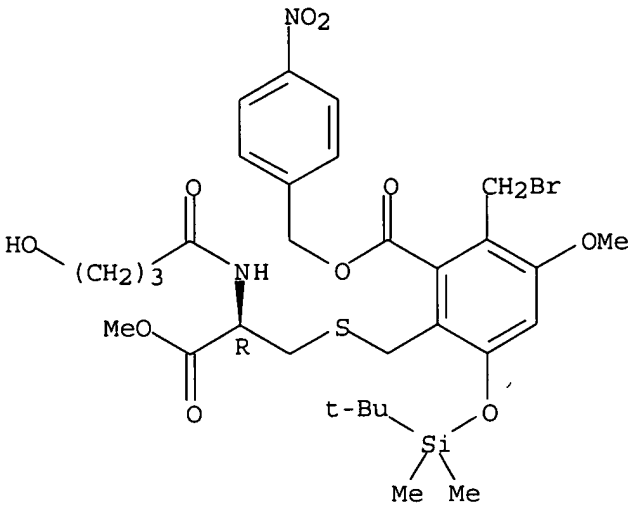
RN 173152-73-3 CAPLUS
CN Benzoic acid, 2-[[(2-amino-3-methoxy-3-oxopropyl)thio]methyl]-6-(bromomethyl)-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-methoxy-, (4-nitrophenyl)methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



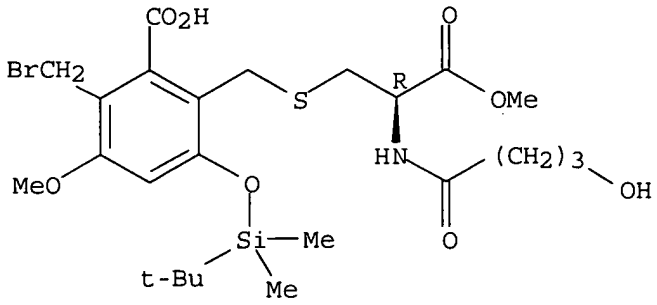
RN 173152-74-4 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[(4-hydroxy-1-oxobutyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-3-methoxy-, (4-nitrophenyl)methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



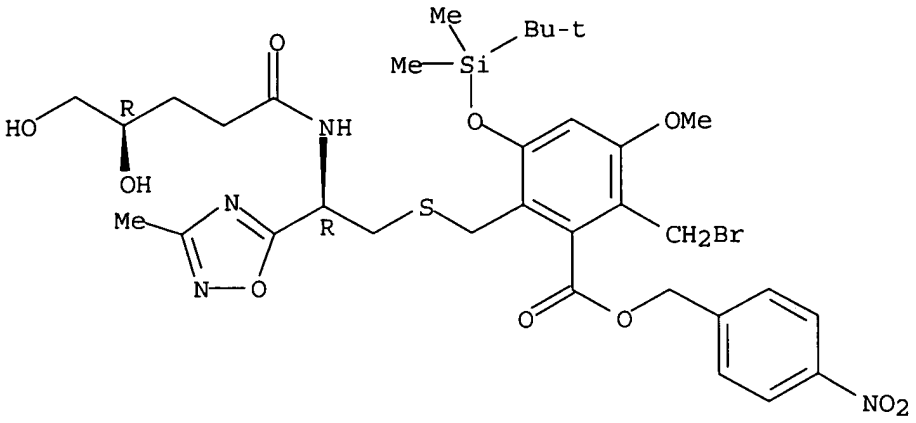
RN 173152-75-5 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[(4-hydroxy-1-oxobutyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-3-methoxy-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



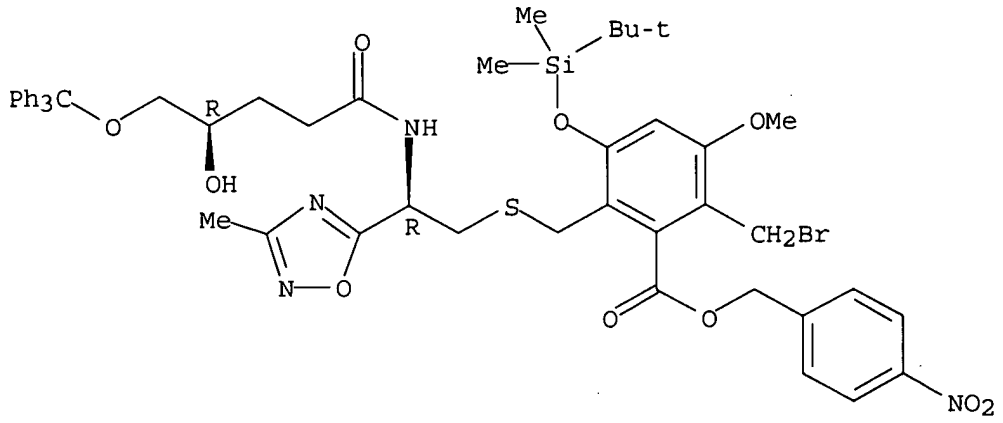
RN 173152-76-6 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-[[[2-[(4,5-dihydroxy-1-oxopentyl)amino]-2-(3-methyl-1,2,4-oxadiazol-5-yl)ethyl]thio]methyl]-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methoxy-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



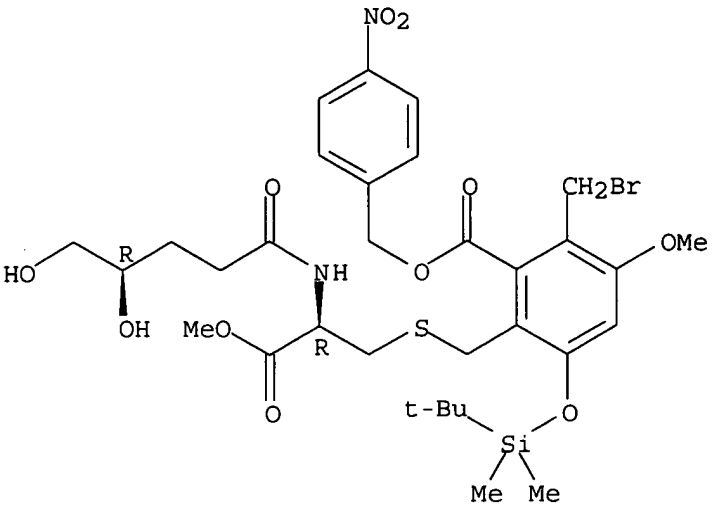
RN 173152-77-7 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[[4-hydroxy-1-oxo-5-(triphenylmethoxy)pentyl]amino]-2-(3-methyl-1,2,4-oxadiazol-5-yl)ethyl]thio]methyl]-3-methoxy-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



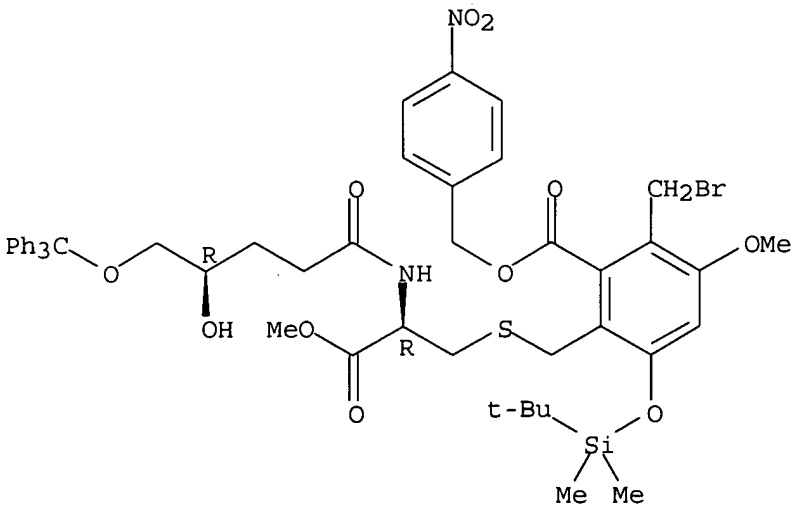
RN 173152-81-3 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-[[[2-[(4,5-dihydroxy-1-oxopentyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3-methoxy-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



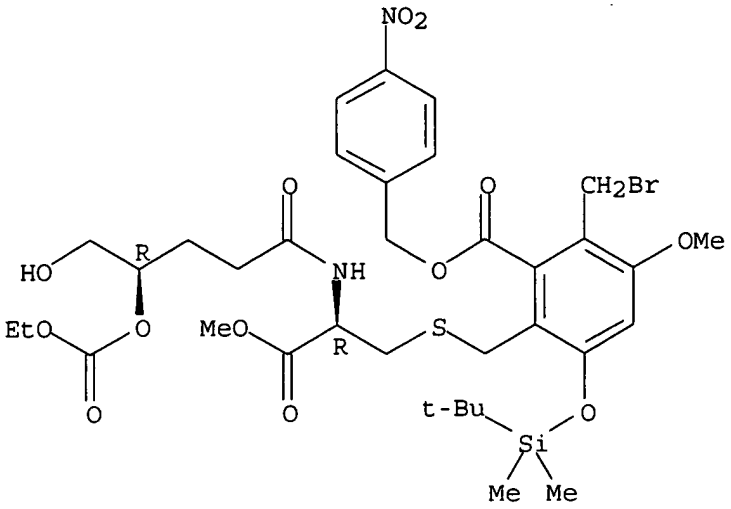
RN 173152-90-4 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[2-[[4-hydroxy-1-oxo-5-(triphenylmethoxy)pentyl]amino]-3-methoxy-3-oxopropyl]thio]methyl]-3-methoxy-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



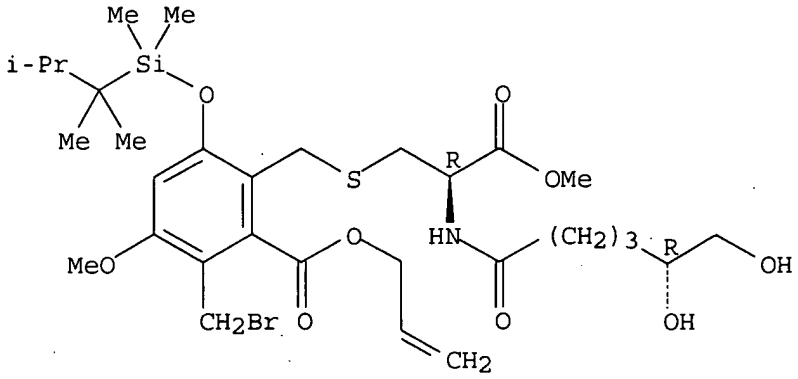
RN 173152-93-7 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[9-(hydroxymethyl)-4-(methoxycarbonyl)-6,11-dioxo-10,12-dioxa-2-thia-5-azatetradec-1-yl]-3-methoxy-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173153-35-0 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-[[[2-[(5,6-dihydroxy-1-oxohexyl)amino]-3-methoxy-3-oxopropyl]thio]methyl]-5-[[dimethyl(1,1,2-trimethylpropyl)silyl]oxy]-3-methoxy-, 2-propenyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173153-79-2 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-[[[3-methoxy-3-oxo-2-[[1-oxo-2-(triphenylmethoxy)propyl]amino]propyl]thio]methyl]-, (4-nitrophenyl)methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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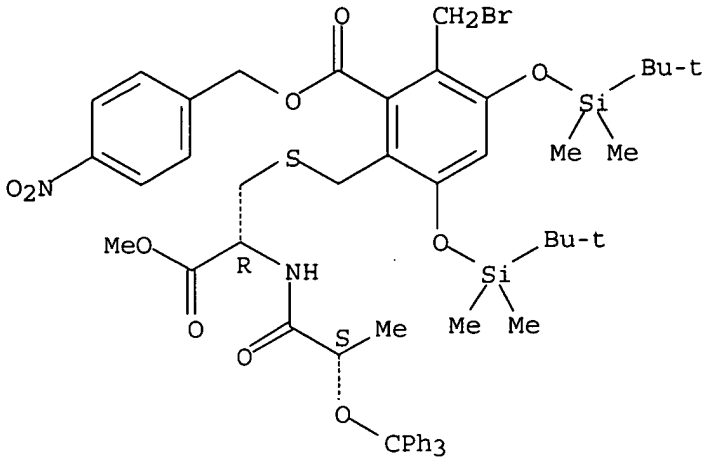

L3 ANSWER 70 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:963356 CAPLUS
DN 124:145548
TI Chemistry and application of phosphonium and arsonium ylides. XX. Synthesis of dimethyl 3-perfluoroalkyl-4-(3-oxo-2-triphenylphosphoranylidenbutanylidene)-2-pentenedioate and its cyclization
AU Ding, Wei-Yu; Cao, Wei-Guo; Yao, Yuan; Zhu, Zhong-Mei
CS Dep. of Chemistry, Shanghai Univ. of Science and Technology, Shanghai, 201800, Peop. Rep. China
SO Chinese Journal of Chemistry (1995), 13(5), 468-74
CODEN: CJOCEV; ISSN: 1001-604X
PB Science Press
DT Journal
LA English
OS CASREACT 124:145548
AB The title compds. were prepared from Me 2-perfluoroalkynoates and Me 5-oxo-4-(triphenylphosphoranylidene)hex-2-enoate. The latter was obtained from Me propynoate and acetylmethylenetriphenylphosphorane. Intramol. elimination of Ph3PO took place when compound the title compds. were heated in aqueous methanol at 115-120°C in sealed tube, yielding di-Me 2-trifluoromethyl-4-methylisophthalate and 5-acetyl-4-hydroxy-2-(heptafluoropropyl)benzoate, resp. The structures of the title compds. were confirmed by IR, MS, 1H NMR, 19F NMR and 13C NMR spectroscopy and elemental analyses. Reaction mechanisms for the fromation of the title compds. were proposed.
IT **170796-03-9P 173383-73-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzoates via cyclization of (perfluoroalkyl)(oxotriphenylphosphoranylidenbutanylidene)pentenedioates)
RN 170796-03-9 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-methyl-2-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

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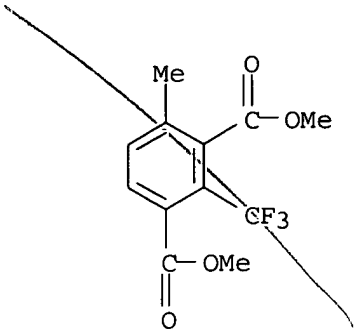
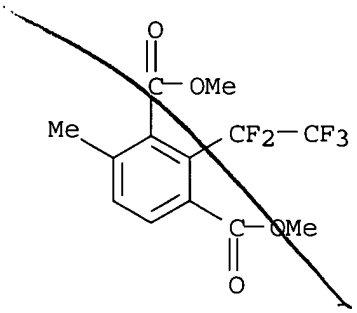
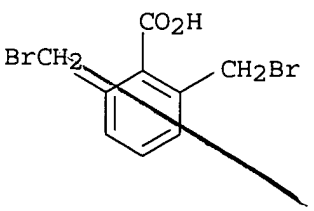


RN 173383-73-8 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-methyl-2-(pentafluoroethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 71 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:761285 CAPLUS
DN 123:339812
TI Sodium sulfide adsorbed on alumina as a reagent for the facile synthesis of 2,11-dithia[3.3]metacyclophanes
AU Bodwell, Graham J.; Houghton, Tom J.; Koury, Holly E.; Yarlagadda, Bala
CS Dep. Chemistry, Memorial Univ. Newfoundland, Newfoundland, A1B 3X7, Can.
SO Synlett (1995), (7), 751-2
CODEN: SYNLES; ISSN: 0936-5214
PB Thieme
DT Journal
LA English
OS CASREACT 123:339812
AB 2,11-Dithia[3.3]metacyclophanes without internal substituents can be prepared rapidly, easily and in moderate yield by using sodium sulfide adsorbed on alumina (Na2S/Al2O3).
IT **56263-54-8**, 2,6-Bis(bromomethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(sodium sulfide adsorbed on alumina as a reagent for synthesis of dithiametacyclophanes)
RN 56263-54-8 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)- (9CI) (CA INDEX NAME)

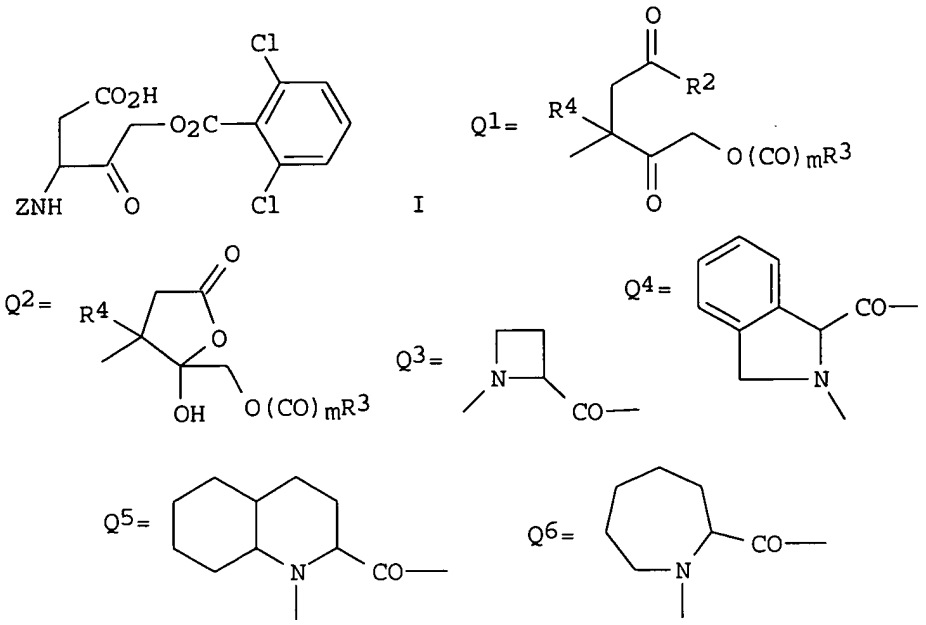


10803578

L3 ANSWER 72 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:735232 CAPLUS
DN 123:170185
TI Preparation of peptide analogs as irreversible interleukin-1β protease inhibitors.
IN Dolle, Roland E.; Osifo, Irennegbe K.; Schmidt, Stanley J.; Hoyer, Denton W.; Ross, Tina M.; Chaturvedula, Prasad; Prouty, Catherine P.; Awad, Mohamed M.; Salvino, Joseph M.; et al.
PA Sterling Winthrop Inc., USA
SO Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 623592	A1	19941109	EP 1994-201161	19940427
	EP 623592	B1	20010627		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CA 2122227	AA	19941030	CA 1994-2122227	19940426
	TW 494094	B	20020711	TW 1994-83103750	19940426
	JP 07025865	A2	19950127	JP 1994-89532	19940427
	AT 202554	E	20010715	AT 1994-201161	19940427
	ES 2160609	T3	20011116	ES 1994-201161	19940427
	PT 623592	T	20011228	PT 1994-201161	19940427
	AU 9460752	A1	19941103	AU 1994-60752	19940428
	AU 676887	B2	19970327		
	IL 109471	A1	19980222	IL 1994-109471	19940428
	FI 9402005	A	19941030	FI 1994-2005	19940429
	NO 9401580	A	19941031	NO 1994-1580	19940429
	HU 68563	A2	19950628	HU 1994-1251	19940429
	US 5985838	A	19991116	US 1996-679350	19960710
	US 6576614	B1	20030610	US 1999-421954	19991020
	GR 3036739	T3	20011231	GR 2001-401596	20010927
	US 2004009923	A1	20040115	US 2003-347641	20030116
PRAI	US 1993-55051	A	19930429		
	US 1995-371723	B1	19950112		
	US 1996-679350	A3	19960710		
	US 1999-421954	A3	19991020		

OS MARPAT 123:170185
GI



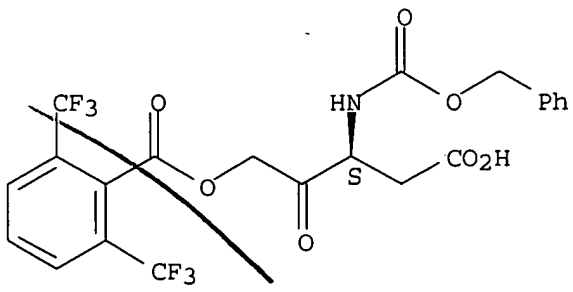
AB R1AnNHY [n = 0-4; Y = Q1, Q2; m = 0,1; R2 = OR6, NR6OR7, NR6R7; R3 = (substituted) Ph, naphthyl; R6, R7 = H, alkyl, PhCH2, cycloalkyl, (hetero)aryl; A = Q3-Q6, other amino acid residue], were prepared Thus, Z-Asp(OtBu)-OH in THF at -15° was treated sequentially with N-methylmorpholine, EtO2CCl, and CH2N2 followed by warming to room temperature The diazoketone solution was treated with HBr/HOAc to give Z-Asp(OtBu)-CH2Br. This was stirred with KF and 2,6-dichlorobenzoic acid in DMF and the condensation product was treated with CF3CO2H in CH2Cl2 to give title compound L-I. The latter inhibited Il-1β protease with IC50 = 0.05 nM.

IT **166388-64-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptide ketone analogs as irreversible interleukin-1β protease inhibitors)

RN 166388-64-3 CAPLUS

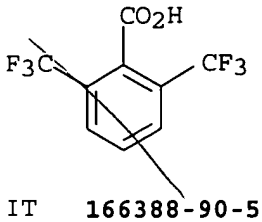
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 4-carboxy-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]butyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



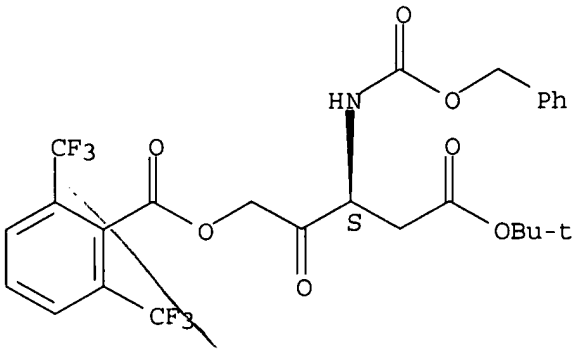
IT **24821-22-5**, 2,6-Ditrifluoromethylbenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptide ketone analogs as irreversible interleukin-1β

protease inhibitors)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



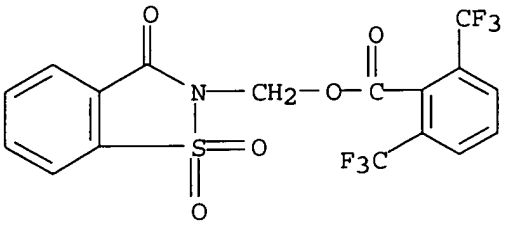
IT **166388-90-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptide ketone analogs as irreversible interleukin-1β protease inhibitors)
RN 166388-90-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 5-(1,1-dimethylethoxy)-2,5-dioxo-3-[[(phenylmethoxy)carbonyl]amino]pentyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

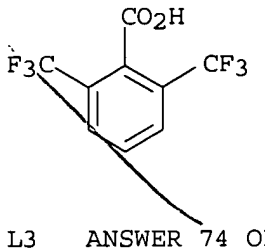


L3 ANSWER 73 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:733809 CAPLUS
DN 123:228044
TI 2,6-Disubstituted Aryl Carboxylic Acids, Leaving Groups "Par Excellence" for Benzisothiazolone Inhibitors of Human Leukocyte Elastase. [Erratum to document cited in CA121:230709]
AU Subramanyam, Chakrapani; Bell, Malcolm R.; Carabateas, Philip; Court, John J.; Dority, John A. Jr.; Ferguson, Edward; Gordon, Robert; Hlasta, Dennis J.; Kumar, Virendra; et al.
CS Department of Medicinal Chemistry, Sterling Winthrop Pharmaceutical Research Division, Collegeville, PA, 19426-0900, USA
SO Journal of Medicinal Chemistry (1995), 38(16), 3188
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The corrected generic structure for compds. 7a-c in table 3 is given. The errors were not reflected in the abstract or the index entries.
IT **142426-83-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

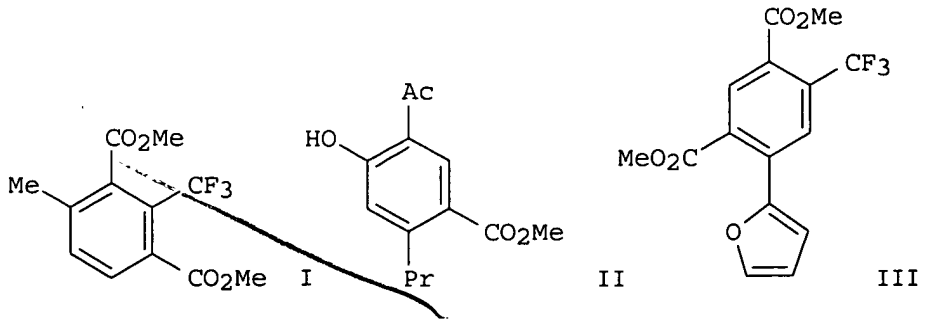
(preparation and inhibition of human leukocyte elastase by (Erratum))
RN 142426-83-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester (9CI) (CA INDEX NAME)



IT **24821-22-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of N-aroyloxymethyl benzisothiazolones (Erratum))
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 74 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:656321 CAPLUS
DN 123:338967
TI Structural determination of polysubstituted benzene derivatives by COLOC NMR technique
AU Yao, Yuan; Shi, Zhijian; Yang, Guojuan
CS Dep. Chem., Shanghai Univ. Sci. Technol., Shanghai, 201800, Peop. Rep. China
SO Bopuxue Zazhi (1995), 12(3), 269-76
CODEN: BOZAE2; ISSN: 1000-4556
PB Zhongguo Kexueyuan Wuhan Wuli Yanjiuso
DT Journal
LA Chinese
GI



I II III

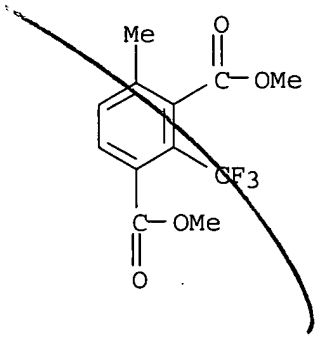
10803578

AB Polysubstituted benzene derivs. I, II, and III were synthesized via acyclic precursors through intramol. Witting reaction. 2D COLOC NMR technique was used to determine the location of each substituent in their structural identification. The difference between the calculated and the measured chemical shift of each aromatic carbon and the 3JCF coupling consts. were discussed.

IT **170796-03-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(structural determination of polysubstituted benzene derivs. by COLOC NMR technique)

RN 170796-03-9 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 4-methyl-2-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 75 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:522755 CAPLUS

DN 122:291211

TI Preparation of pyrethrinoid esters derived from 6-trifluoromethylbenzyl alcohol as pesticides

IN Babin, Didier; Benoit, Marc; Bouchet, Raphael; Demoute, Jean Pierre

PA Roussel-UCLAF, Fr.

SO Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 638542	A1	19950215	EP 1994-401804	19940804
	EP 638542	B1	19990421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE				
	FR 2708600	A1	19950210	FR 1993-9653	19930805
	FR 2708600	B1	19950915		
	JP 07069989	A2	19950314	JP 1994-200316	19940803
	CA 2129484	AA	19950206	CA 1994-2129484	19940804
	AU 9468882	A1	19950216	AU 1994-68882	19940804
	BR 9403169	A	19950411	BR 1994-3169	19940804
	HU 67967	A2	19950529	HU 1994-2281	19940804
	CN 1108237	A	19950913	CN 1994-115029	19940804
	AT 179161	E	19990515	AT 1994-401804	19940804
	US 5504112	A	19960402	US 1995-441331	19950515
PRAI	FR 1993-9653	A	19930805		
	US 1994-280798	B1	19940726		

OS MARPAT 122:291211

GI

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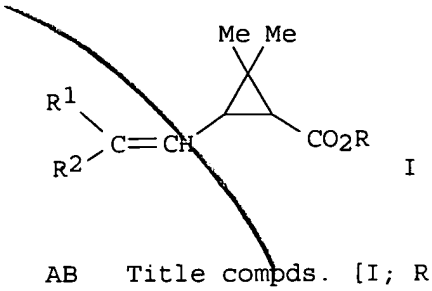


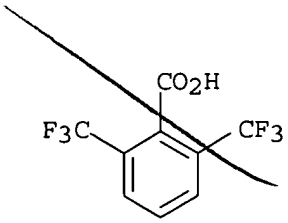
I

AB Title compds. [I; R = 2,6-Y(F3C)C6H3CHX; R1 = H and R2 = halo; R1,R2 = halo; R1 = R2 = CF3; X = H, alk(en)yl, (ar)alkynyl, cyano; Y = halo, CH2F, CHF2, CF3] were prepared as pesticides (no data). Thus, (1R)-cis-I (R1 = F, R2 = Cl)(II; R = H) was esterified by 2,6-(F3C)2C6H3CH2OH (preparation given) to give II [R = 2,6-(F3C)2C6H3CH2].

IT **24821-22-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrethrinoid esters derived from 6-trifluoromethylbenzyl alc. as pesticides)

RN 24821-22-5 CAPLUS

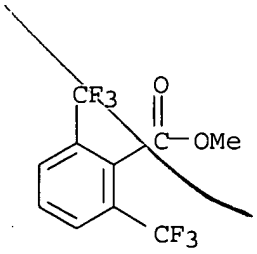
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



IT **34060-79-2P**, Benzoic acid, 2,6-Bis(trifluoromethyl)-, methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrethrinoid esters derived from 6-trifluoromethylbenzyl alc. as pesticides)

RN 34060-79-2 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 76 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:408386 CAPLUS

DN 123:143928

TI 2-saccharinylmethyl benzoates, their preparation and use for the treatment of degenerative diseases

IN Subramanyam, Chakrapani; Bell, Malcolm R.

PA Sterling Winthrop, Inc., USA

SO U.S., 48 pp. cont.-in-part of U.S. 5,250,696.
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 7

10803578

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5306818	A	19940426	US 1992-965593	19921023
	US 5128339	A	19920707	US 1991-782016	19911024
	IL 114773	A1	19961205	IL 1991-114773	19911031
	US 5250696	A	19931005	US 1992-860340	19920330
	NO 9202976	A	19920504	NO 1992-2976	19920728
	NO 301116	B1	19970915		
	AU 9344526	A1	19940505	AU 1993-44526	19930810
	AU 679446	B2	19970703		
	US 5380737	A	19950110	US 1993-113508	19930827
	US 5512589	A	19960430	US 1993-116416	19930903
	CA 2105731	AA	19940424	CA 1993-2105731	19930908
	JP 06211849	A2	19940802	JP 1993-231485	19930917
	IL 107315	A1	19990312	IL 1993-107315	19931018
	EP 594257	A1	19940427	EP 1993-202925	19931020
	EP 594257	B1	19960710		
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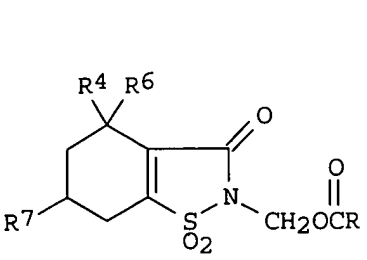
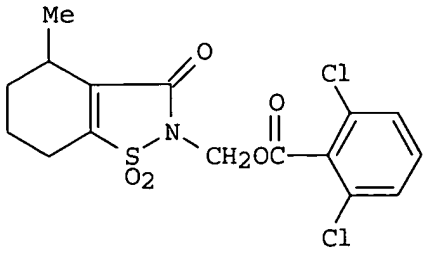
	AT 140227	E	19960715	AT 1993-202925	19931020
	ES 2092751	T3	19961201	ES 1993-202925	19931020
	FI 9304675	A	19940424	FI 1993-4675	19931022
	NO 9303817	A	19940425	NO 1993-3817	19931022
	NO 304375	B1	19981207		
	HU 68879	A2	19950828	HU 1993-3009	19931022
	HU 70756	A2	19951030	HU 1994-569	19940225
	HU 70764	A2	19951030	HU 1994-580	19940225
	US 5464852	A	19951107	US 1994-289113	19940811
	FI 9404968	A	19941021	FI 1994-4968	19941021
	US 5578623	A	19961126	US 1995-445240	19950519
	US 5597841	A	19970128	US 1995-445118	19950519
	FI 9600490	A	19960202	FI 1996-490	19960202
	FI 103115	B1	19990430		
	US 5773456	A	19980630	US 1996-719216	19960925
PRAI	US 1990-608068	B2	19901101		
	US 1991-782016	A3	19911024		
	US 1992-860340	A2	19920330		
	US 1989-347125	B2	19890504		
	US 1989-347126	B2	19890504		
	US 1990-514920	A	19900426		
	HU 1991-3430	A	19911031		
	IL 1991-99913	A3	19911031		
	FI 1991-5163	A	19911101		
	NO 1991-4288	A1	19911101		
	US 1991-793035	B1	19911115		
	US 1992-965593	A	19921023		
	US 1993-113508	A3	19930827		
	US 1993-116416	A3	19930903		
	US 1994-289113	A3	19940811		
	FI 1994-4968	A	19941021		
	US 1995-445240	A3	19950519		
OS	MARPAT 123:143928				
GI					

10803578



I



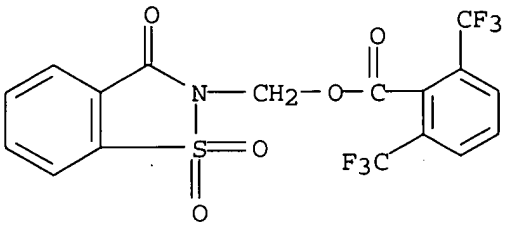
II

AB The title compds. I (R = aryl; R4 = H, alkyl, phenyl; R6 H H, alkyl, etc.; R7 = H, alkoxy) were disclosed. I are useful in the treatment of degenerative diseases. A specifically claimed compound, (4-methyl-4,5,6,7-tetrahydro-2-saccharinyl)methyl 2,6-dichlorobenzoate [i.e. 2,6-dichlorobenzoic acid (4,5,6,7-tetrahydro-4-methyl-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester S,S-dioxide] (II) was prepared

IT **142426-83-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, for treatment of degenerative diseases)

RN 142426-83-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 77 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:314941 CAPLUS

DN 122:133157

TI Towards structurally responsive synthetic macrocyclic receptors for acetylcholine

AU Parker, David; Rosser, Mark

CS Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1995), (1), 85-9
CODEN: JCPKBH; ISSN: 0300-9580

PB Royal Society of Chemistry

DT Journal

LA English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

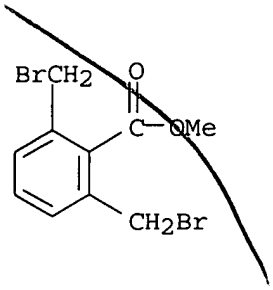
AB The synthesis and complexation behavior of structurally related neutral and ionic cyclophanes are reported. A neutral pyridino-cyclophane (I) selectively mediates transport of acetylcholine while ionic receptors

incorporating both a pyridine moiety and a carboxyphenyl group, e.g., II, form stronger complexes in aqueous THF as revealed by 1H NMR spectroscopy. These ionic receptors form 1:1 complexes with the substrate.

IT **56263-51-5**, Methyl 2,6-bis(bromomethyl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthetic macrocyclic receptors for acetylcholine)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 78 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:270974 CAPLUS

DN 122:240406

TI Functionalized depsipeptides, substrates and inhibitors of β-lactamases and DD-peptidases

AU Cabaret, D.; Liu, J.; Wakselman, M.; Pratt, R. F.; Xu, Y.

CS CERCOA, CNRS, Thiais, F-94320, Fr.

SO Bioorganic & Medicinal Chemistry (1994), 2(8), 757-71
CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier

DT Journal

LA English

OS CASREACT 122:240406

AB A series of derivs. of Ph phenylacetylglycinates (aryl phenaceturates) with a carboxylate substituent meta to the oxygen of the phenoxide leaving group and a functionalized methylene group in the ortho- or para-position have been synthesized. These mols. possess a latent o- or p-quinone methide electrophile which could be unmasked during enzymic turnover and could react with an active site nucleophile. This chemical does seem to occur in solution where a common hydrolysis product, independent of the benzylic leaving group, presumably o- or p-hydroxymethylphenol, was observed These depsipeptides are substrates of class A and C β-lactamases, particularly of the latter, comparable with the parent m-carboxyphenyl phenaceturate. They also have modest inhibitory activity against these enzymes and against the serine DD-peptidase of Streptomyces R61. The inhibition of a class C β-lactamase was turnover dependent, as expected of mechanism-based inhibitor, but the small leaving group dependence of the inhibition suggested that the quinone methide, if it was in fact responsible for the inhibition, was generated in solution subsequent to release of the product phenol from the active site.

IT **162213-90-3P 162213-92-5P 162213-93-6P**
162213-99-2P 162214-05-3P 162214-11-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(functionalized depsipeptides, substrates and inhibitors of β-lactamases and DD-peptidases)

RN 162213-90-3 CAPLUS

CN Benzoic acid, 2-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methyl]-5-hydroxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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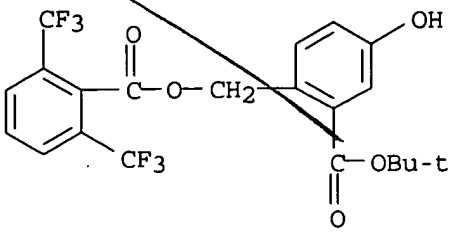
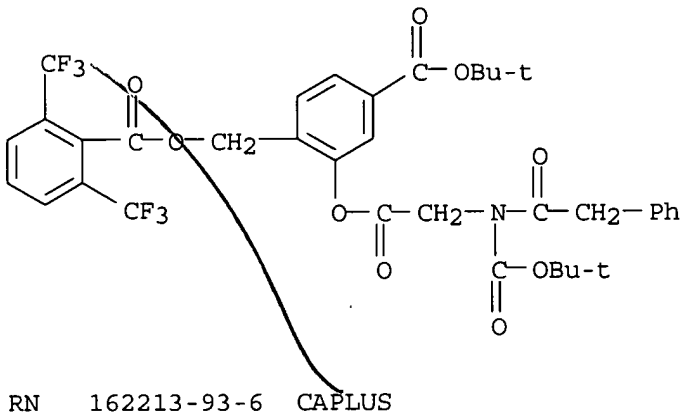
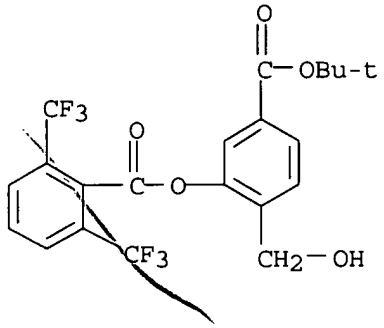


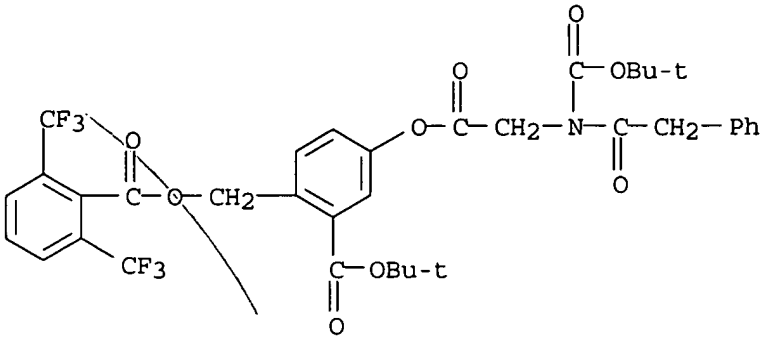
RN 162213-92-5 CAPLUS
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-(phenylacetyl)-, 2-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methyl]-5-[(1,1-dimethylethoxy)carbonyl]phenyl ester (9CI) (CA INDEX NAME)



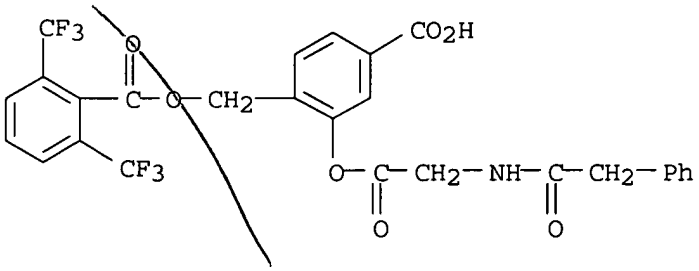
RN 162213-93-6 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 5-[(1,1-dimethylethoxy)carbonyl]-2-(hydroxymethyl)phenyl ester (9CI) (CA INDEX NAME)



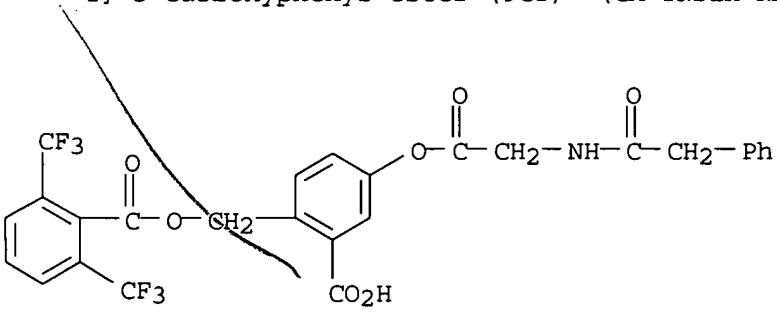
RN 162213-99-2 CAPLUS
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-(phenylacetyl)-, 4-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methyl]-3-[(1,1-dimethylethoxy)carbonyl]phenyl ester (9CI) (CA INDEX NAME)



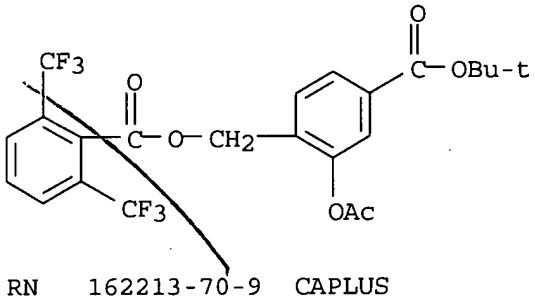
RN 162214-05-3 CAPLUS
CN Glycine, N-(phenylacetyl)-, 2-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methy l]-5-carboxyphenyl ester (9CI) (CA INDEX NAME)



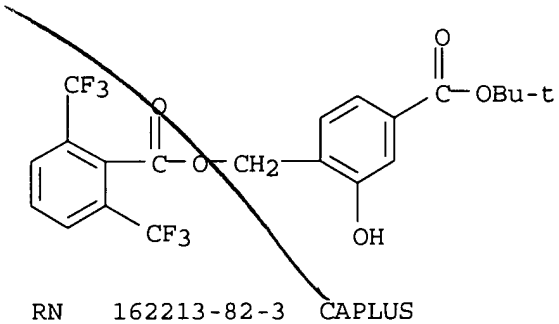
RN 162214-11-1 CAPLUS
CN Glycine, N-(phenylacetyl)-, 4-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methy l]-3-carboxyphenyl ester (9CI) (CA INDEX NAME)



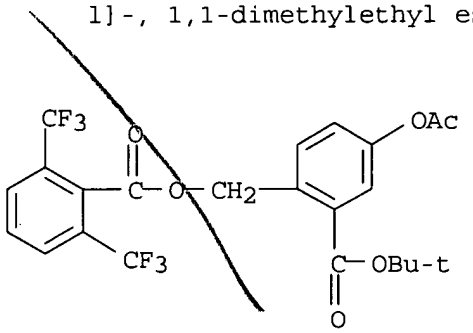
IT **162213-64-1P 162213-70-9P 162213-82-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; functionalized depsipeptides, substrates and inhibitors of β-lactamases and DD-peptidases)
RN 162213-64-1 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, [2-(acetyloxy)-4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)



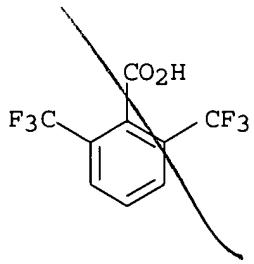
RN 162213-70-9 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, [4-[(1,1-dimethylethoxy)carbonyl]-2-hydroxyphenyl]methyl ester (9CI) (CA INDEX NAME)



RN 162213-82-3 CAPLUS
CN Benzoic acid, 5-(acetyloxy)-2-[[[2,6-bis(trifluoromethyl)benzoyl]oxy]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



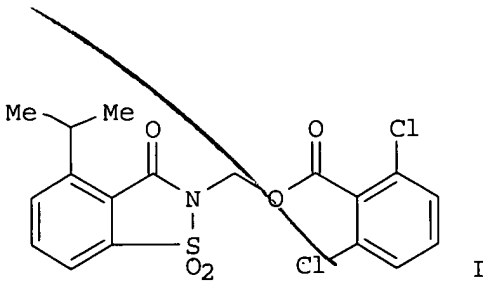
IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; functionalized depsipeptides, substrates and inhibitors of β-lactamases and DD-peptidases)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 79 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:630709 CAPLUS
DN 121:230709
TI 2,6-Disubstituted Aryl Carboxylic Acids, Leaving Groups "Par Excellence" for Benzisothiazolone Inhibitors of Human Leukocyte Elastase

10803578

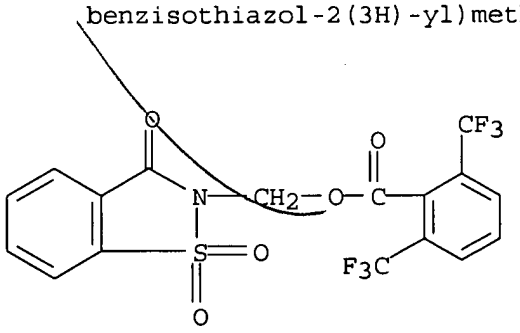
AU Subramanyam, Chakrapani; Bell, Malcolm R.; Carabateas, Philip; Court, John J.; Dority, John A. Jr.; Ferguson, Edward; Gordon, Robert; Hlasta, Dennis J.; Kumar, Virendra; et al.
CS Department of Medicinal Chemistry, Sterling Winthrop Pharmaceutical Research Division, Collegeville, PA, 19426-0900, USA
SO Journal of Medicinal Chemistry (1994), 37(17), 2623-6
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



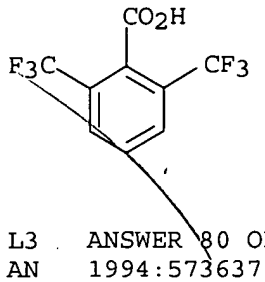
I

AB A number of N-aroyloxymethyl benzisothiazolones were prepared and found to be potent mechanism based inhibitors of human elastase (HLE). Of the various 2,6-disubstituted aryl carboxylic acids attached as leaving groups onto N-Me of the benzisothiazolone nucleus, 2,6-dichlorobenzoic acid was the best. This finding in conjunction with a C4 iso-Pr substituent led to compound I (WIN 62814) with Ki = 0.03 nM. Introduction of polar substituent at C3' led to the discovery of compound I.HCl (II) (WIN 63110) the most potent inhibitor in this series with Ki = 0.007 nM and ED50 = 1.0 mg/kg. II is the most potent (highest inactivation rate) small mol. inhibitor ever reported for a serine protease.

IT **142426-83-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of human leukocyte elastase by)
RN 142426-83-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester (9CI) (CA INDEX NAME)

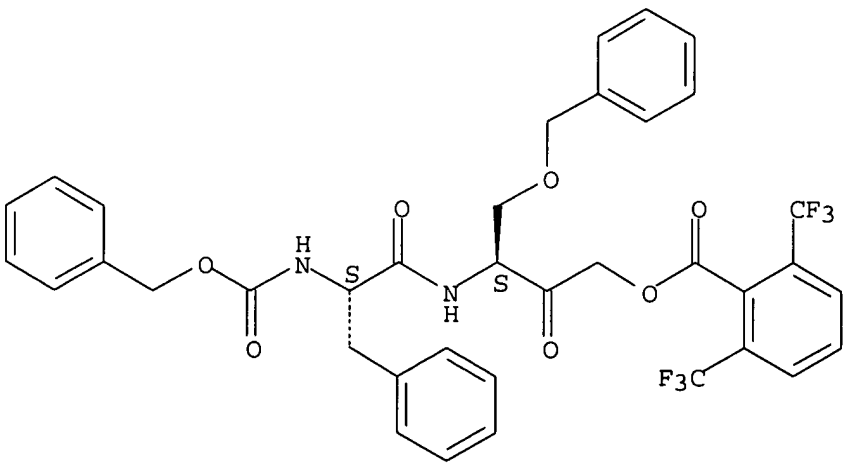


IT **24821-22-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of N-aroyloxymethyl benzisothiazolones)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 80 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:573637 CAPLUS
DN 121:173637
TI Potent inactivation of cathepsins S and L by peptidyl (acyloxy)methyl ketones
AU Bromme, Dieter; Smith, Roger A.; Coles, Peter J.; Krischke, Heidrun; Storer, Andrew C.; Krantz, Allen
CS Biotechnol. Res. Inst., Natl. Res. Counc. Canada, Montreal, QC, H4P 2R2, Can.
SO Biological Chemistry Hoppe-Seyler (1994), 375(5), 343-7
CODEN: BCHSEI; ISSN: 0177-3593
DT Journal
LA English
AB Peptidyl (acyloxy)methyl ketones (Z-Aa-Aa-CH2-O-CO-R), a new class of irreversible inhibitors whose chemical reactivity can be modulated by varying the substitution pattern of the carboxylate leaving group, are shown to be extremely potent inactivators of the lysosomal cysteine proteinases cathepsin L and cathepsin S. The highest k2/Ki values measured were found to exceed 106 m-1s-1 for both cathepsin L and cathepsin S. The rate of inactivation can be controlled by varying the dipeptidyl moiety or the carboxylate leaving group, with the second-order rate consts. for both enzymes strongly dependent on the pKa values of the leaving group. The specificities of the cathepsins S and L reveal a different selectivity towards the nature of substitution of the aryl P' leaving group of the inhibitor. This new inhibitor class opens the possibility of the design of selective and specific inhibitors for lysosomal cysteine proteinases.
IT **115186-02-2 115186-03-3 118237-64-2**
RL: BIOL (Biological study)
(cathepsin S of human and cathepsin L inhibition by, structure in relation to)
RN 115186-02-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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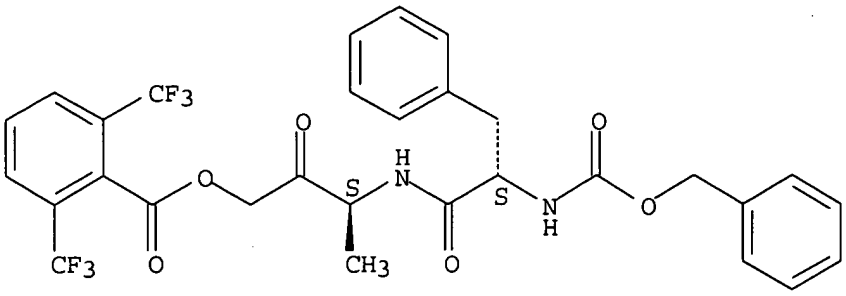
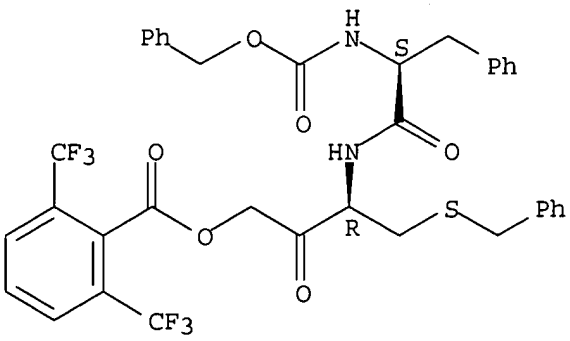
RN 115186-03-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



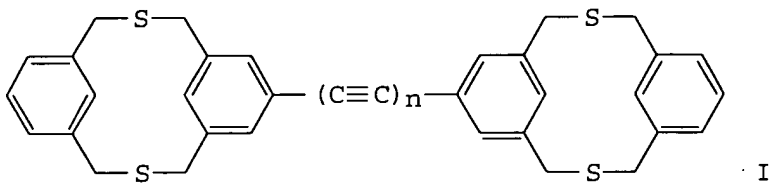
RN 118237-64-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-[(phenylmethyl)thio]butyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

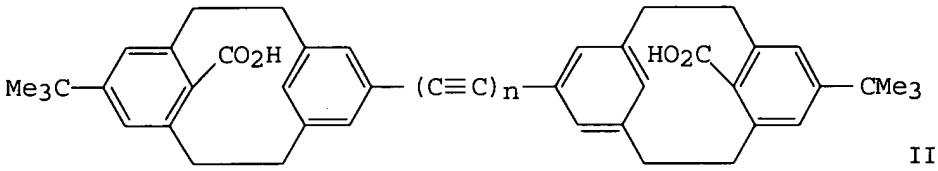


L3 ANSWER 81 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:508739 CAPLUS
DN 121:108739
TI Molecular tweezers from cyclophane building blocks
AU Guether, Ralf; Nieger, Martin; Rissanen, Kari; Voegtle, Fritz
CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, 53121, Germany
SO Chemische Berichte (1994), 127(4), 743-57
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
GI

10803578



I

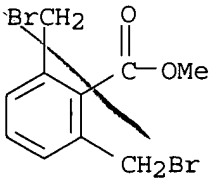


II

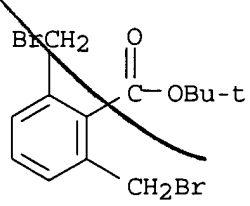
AB Mol. tweezer compds. I and II (n = 0-2) with convergent carboxyl groups are prepared from suitable functionalized [2.2]- and dithia[3.3]metacyclophane building blocks by using several multistep strategies. The C-C coupling of two cyclophanes according to the Hagihara method leads to the alkyne-spacered double cyclophanes. These new preorganized, acyclic host compds. of the cyclophane-type react as mol. tweezers and can selectively grasp guest mols. and bind them strongly. X-ray analyses underline the syn conformations of I and the anti conformation of II.

IT **56263-51-5 56263-53-7 119319-00-5 156597-75-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of alkynylbis(metacyclophane) mol. tweezers)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

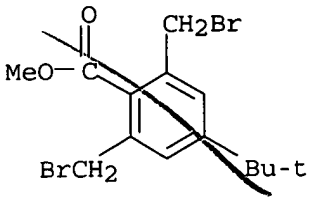


RN 56263-53-7 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

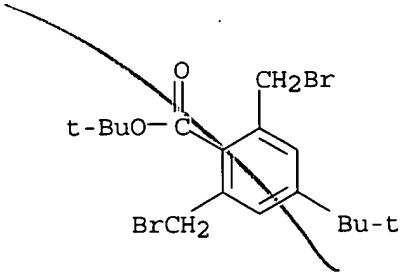


RN 119319-00-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)

10803578



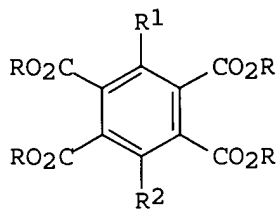
RN 156597-75-0 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



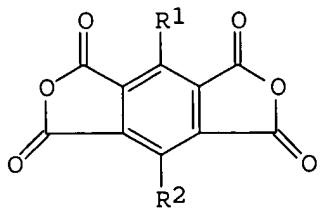
L3 ANSWER 82 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:323553 CAPLUS
DN 120:323553
TI Preparation of pyromellitic acid derivatives and anhydrides thereof
IN Fujiwara, Koji; Kudo, Masaaki; Akita, Takayuki
PA Nihon Nohyaku Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06041016	A2	19940215	JP 1993-145601	19930525
	JP 3605732	B2	20041222		
PRAI	JP 1992-158743	A1	19920526		

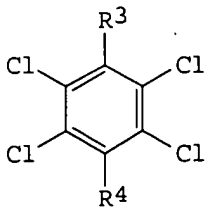
OS CASREACT 120:323553; MARPAT 120:323553
GI



I



II



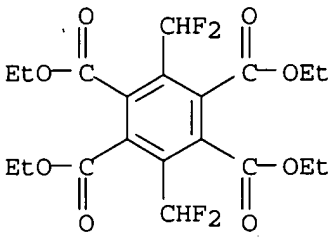
III

AB Pyromellitic acid derivs. [I; R = H, alkyl; R1, R2 = lower (fluoro)alkyl; provided that R1 = R2 ≠ CF3] and anhydrides thereof (II; R1, R2 = same as above) which can be used as monomers for polyimides (no data), are prepared via alkoxycarbonylation of tetrachlorobenzene derivs. [III; R3, R4 = H, cyano, lower (halo)alkyl or (halo)alkoxy] with CO and ROH (R = lower alkyl) in the presence of a Pd compound, a phosphine compound, and a base to give pyromellitic acid esters I [R = lower alkyl; R1, R2 = H, cyano, lower (halo)alkyl or (halo)alkoxy]. Thus, III (R3 = R4 = CHCl2), TaCl5, and HF were heated at 160° for 5 h in a Hastelloy autoclave to give 52.5% III (R3 = R4 = CHF2) which was reacted with CO (40 kg/cm2) and EtOH in the presence of [Ph3P]2PdCl2 and Na2CO3 in toluene in an autoclave at 200° to give 24.1% triester I (R = Et, R1 = R2 = CHF2). The latter compound was saponified with aqueous 85% KOH in EtOH under reflux, cooled, and acidified with HCl to give 66.7% pyromellitic acid I (R = H, R1 = R2 = CHF2) which was refluxed with Ac2O to give 55.7% dianhydride II (R1 = R2 = CHF2).

IT **155105-22-9P**, Tetraethyl 1,4-bis(difluoromethyl)-2,3,5,6-benzenetetracarboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)

RN 155105-22-9 CAPLUS

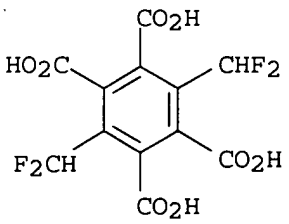
CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(difluoromethyl)-, tetraethyl ester (9CI) (CA INDEX NAME)



IT **155105-23-0P**, 1,4-Bis(difluoromethyl)-2,3,5,6-benzenetetracarboxylic acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and treatment of, with acetic anhydride, pyromellitic anhydride derivative from)

RN 155105-23-0 CAPLUS

CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(difluoromethyl)- (9CI) (CA INDEX NAME)



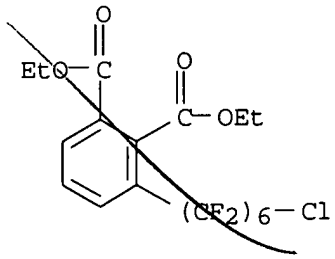
L3 ANSWER 83 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:322835 CAPLUS

DN 120:322835

10803578

TI Perfluoroalkylation of aromatics
AU Huang, Weiyuan; Ying, Weiwen; Zhang, Hanzhong; Liu, Jintao
CS Shanghai Inst. Org. Chem., Chin. Acad. Sci., Shanghai, 200032, Peop. Rep. China
SO Chinese Journal of Chemistry (1993), 11(3), 272-9
CODEN: CJOCEV; ISSN: 1001-604X
DT Journal
LA English
OS CASREACT 120:322835
AB Several methods for the perfluoroalkylation of aroms. were reported. Both perfluoroalkanesulfonyl bromide/benzoyl peroxide and perfluoroalkanesulfinate/oxidant systems were efficient reagents for the introduction of a perfluoroalkyl group onto various aromatic nuclei. In a two-phase solvent system with tetraalkylammonium salt as phase-transfer catalyst, reaction of perfluoroalkyl iodide and aroms. in the presence of sodium dithionite gave perfluoroalkyl aroms. and/or addition-dimerization products.
IT **155367-67-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by perfluoroalkylation of aromatic compound, method for)
RN 155367-67-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(6-chloro-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl)-, diethyl ester (9CI) (CA INDEX NAME)



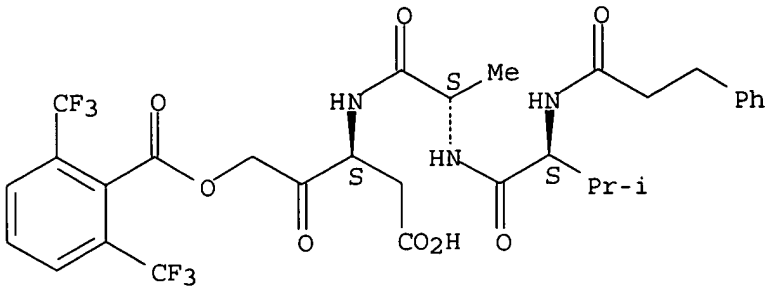
L3 ANSWER 84 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:264340 CAPLUS
DN 120:264340
TI Inactivation of Interleukin-1β Converting Enzyme by Peptide (Acyloxy)methyl Ketones
AU Thornberry, Nancy A.; Peterson, Erin P.; Zhao, Justin J.; Howard, Andrew D.; Griffin, Patrick R.; Chapman, Kevin T.
CS Department of Enzymology Medicinal Chemical Research, Merck Research Laboratories, Rahway, NJ, 07065, USA
SO Biochemistry (1994), 33(13), 3934-40
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB Interleukin-1β converting enzyme (ICE) is a cysteine protease in monocytes that is essential for the proteolytic activation of interleukin-1β, an important mediator of inflammation. Peptide (acyloxy)methyl ketones designed with the appropriate peptide recognition sequence (Ac-Tyr-Val-Ala-Asp-CH2OC(O)Ar) are potent, competitive, irreversible inhibitors. Mass spectrometry and sequence anal. indicate that inactivation proceeds through expulsion of the carboxylate leaving group to form a thiomethyl ketone with the active site Cys285. The second-order inactivation rate is independent of leaving group pKa, with an approx. value of 1 + 106 M-1 s-1. This rate constant is directly proportional to the reaction macroviscosity, indicating that the rate-limiting step in inactivation is association of enzyme and inhibitor,

rather than any bond-forming reactions. Affinity labeling of THP.1 monocytic cell cytosol with a biotinylated tetrapeptide (acyloxy)methyl ketone for 28 half-lives resulted in labeling of only the converting enzyme, demonstrating the selectivity of these inhibitors. These inhibitors are relatively inert toward other bionucleophiles such as glutathione (<5 + 10-4 M-1 s-1), making them excellent candidates for in vivo studies of enzyme inhibition.

IT **151272-16-1P 154674-82-5P 154719-26-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and human interleukin-1β-converting enzyme inhibition by, structure in relation to)

RN 151272-16-1 CAPLUS
CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

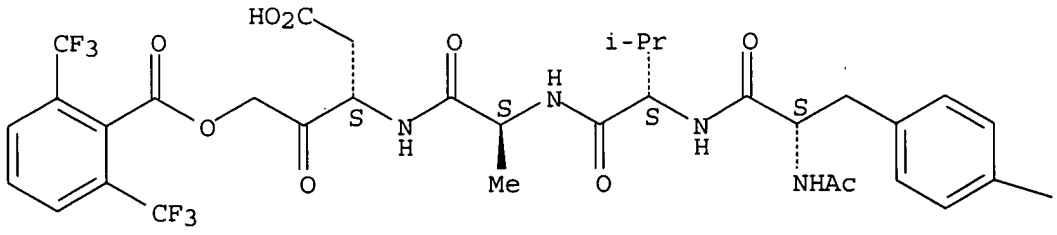
Absolute stereochemistry.



RN 154674-82-5 CAPLUS
CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



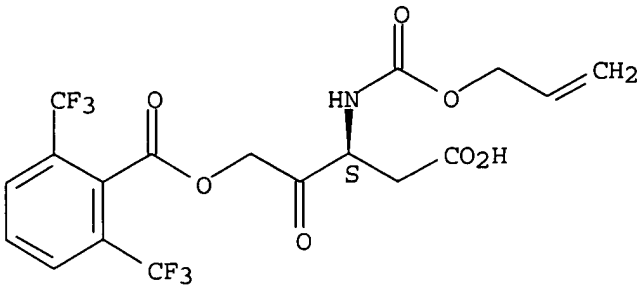
PAGE 1-B

RN 154719-26-3 CAPLUS

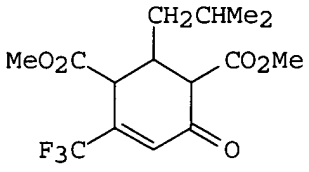
10803578

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (3S)-4-carboxy-2-oxo-3-[[(2-propenyloxy)carbonyl]amino]butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

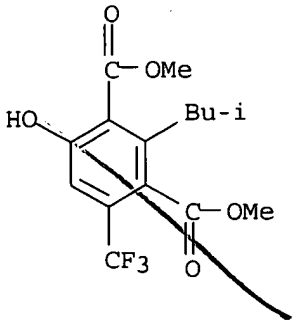


L3 ANSWER 85 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:244265 CAPLUS
DN 120:244265
TI Annulation with methyl 4-(triphenylphosphoranylidene)acetoacetate. Application to the synthesis of a 1,3-benzenedicarboxylate derivative
AU Hegde, S. G.; Bryant, R. D.
CS New Prod. Div., Agric. Group of Monsanto, St. Louis, MO, 63167, USA
SO Synthetic Communications (1993), 23(19), 2753-60
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
OS CASREACT 120:244265
GI

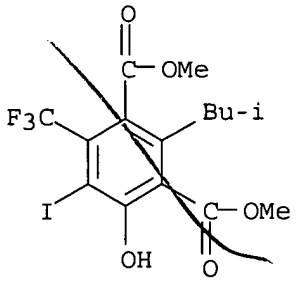


I

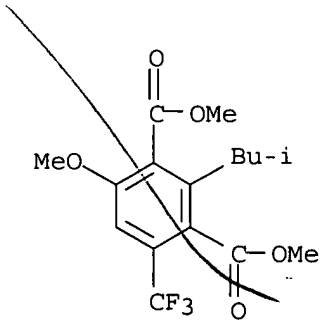
AB Cyclohexenone I was prepared via an annulation reaction of 4-(triphenylphosphoranylidene)acetoacetate Ph3P:CHCOCH2CO2Me and aromatization of I to a 1,3-benzenedicarboxylate derivative
IT **153706-53-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 153706-53-7 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-hydroxy-2-(2-methylpropyl)-6-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT **153706-54-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of, deiodination during)
RN 153706-54-8 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-hydroxy-5-iodo-2-(2-methylpropyl)-6-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT **153706-50-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 153706-50-4 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 4-methoxy-2-(2-methylpropyl)-6-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



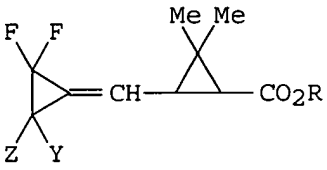
L3 ANSWER 86 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:134869 CAPLUS
DN 120:134869
TI Derivatives of 2,2-dimethyl-3-[(2,2-difluorocyclopropylidene)-methyl]cyclopropanecarboxylic acid, process for their preparation and their use as pesticides
IN Babin, Didier; Benoit, Marc; Demoute, Jean Pierre; Pilorge, Fabienne;

10803578

Reinier, Nicole
PA Roussel-UCLAF, Fr.
SO Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 554167	A1	19930804	EP 1993-400193	19930127
R: CH, DE, FR, GB, IT, LI, NL				
FR 2686602	A1	19930730	FR 1992-865	19920128
FR 2686602	B1	19940311		
US 5340835	A	19940823	US 1993-5603	19930119
JP 05310641	A2	19931122	JP 1993-27134	19930125
PRAI FR 1992-865	A	19920128		

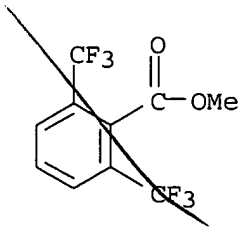
OS MARPAT 120:134869
GI



I

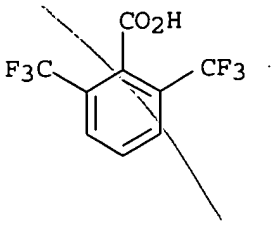
AB The title compds. I (Y, Z = H, halo, CF3, alkyl, etc.; R = alkyl, or a moiety resulting from an alc. used in the synthesis of pyrethrinoid esters), useful as pesticides, were prepared Esterification of [1R-[1α,3α(E)]]-I (Z = Y = R = H) using 2,3,5,6-tetrafluorobenzyl alc. gave [1R-[1α,3α(E)]]-I (Z = Y = H; R = 2,3,5,6-tetrafluorophenylmethyl) (II). II at 10 ppm gave good insecticidal activity against Diabrotica. Formulations containing I are given.

IT **34060-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of pesticide)
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of pesticide)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

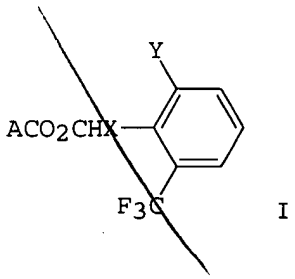
10803578



L3 ANSWER 87 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:77487 CAPLUS
DN 120:77487
TI Pyrethrinoid esters derived from 6-trifluoromethyl benzyl alcohol, process for their preparation and their use as pesticides
IN Babin, Didier; Benoit, Marc; Demoute, Jean Pierre
PA Roussel-UCLAF, Fr.
SO Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 557192	A1	19930825	EP 1993-400404	19930218
	EP 557192	B1	19960821		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE				
	FR 2687666	A1	19930827	FR 1992-2010	19920221
	BR 9300623	A	19931019	BR 1993-623	19930218
	JP 06041015	A2	19940215	JP 1993-51260	19930218
	AT 141586	E	19960915	AT 1993-400404	19930218
	ES 2090898	T3	19961016	ES 1993-400404	19930218
	AU 9333160	A1	19930826	AU 1993-33160	19930219
	AU 663557	B2	19951012		
	HU 64008	A2	19931129	HU 1993-455	19930219
	CN 1075473	A	19930825	CN 1993-101823	19930220
	US 5420159	A	19950530	US 1994-312116	19940926
	US 5574194	A	19961112	US 1995-540083	19951006
PRAI	FR 1992-2010	A	19920221		
	US 1993-17630	B1	19930212		
	US 1994-312116	A3	19940926		
	US 1995-395626	B3	19950128		

OS MARPAT 120:77487
GI

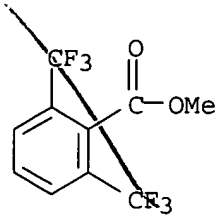


I

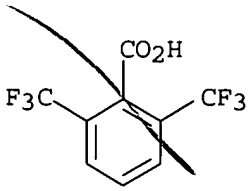
AB The title compds. I [X = H, alkyl, alkenyl, alkynyl, etc.; Y = H, CH2F, CHF2, CF3: A = residue of an acid used in pyrethrinoids (details on A are given)] were prepared I are prepared by reaction of trifluoromethylbenzyl alc. derivs. with the appropriate cyclopropanecarboxylic acids in the presence of dicyclohexylcarbodiimide and 4-dimethylaminopyridine. I at 1 ppm show good activity against Diabrotica. Formulations containing I are given.

10803578

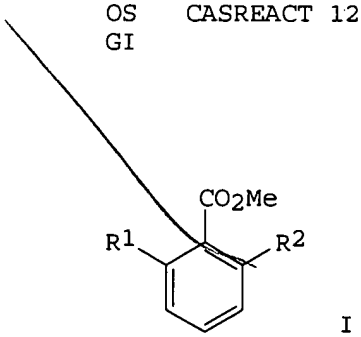
IT **34060-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of insecticide)
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of insecticide)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 88 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:76981 CAPLUS
DN 120:76981
TI Phosphonium and arsonium ylides. XVII. A facile synthesis of methyl 2,6-bis(perfluoroalkyl)benzoates via acyclic precursors
AU Ding, Weiyu; Cao, Weiguo; Xu, Zhenrong; Shi, Zhijian; Yao, Yuan
CS Dep. Chem., Shanghai Univ. Sci. Technol., Shanghai, 201800, Peop. Rep. China
SO Chinese Journal of Chemistry (1993), 11(1), 81-5
CODEN: CJOCEV; ISSN: 1001-604X
DT Journal
LA English
OS CASREACT 120:76981
GI



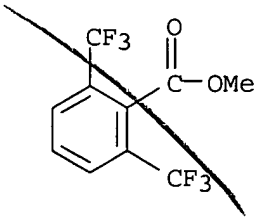
I

AB The title compds. I (R1, R2 = perfluoroalkyl groups, e.g., CF3, C2F5, n-C3F7) were prepared in 82-94% yield via intramol. Wittig reaction of Me 3-perfluoroalkyl-6-perfluoroacetyl-2-triphenylphosphoranylidenehexa-3,5-

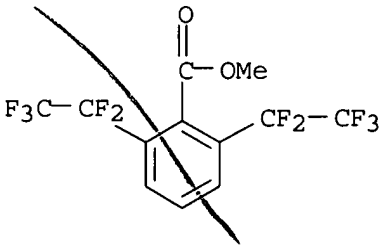
dienoates Ph3P:C(CO2Me)CR2:CHCH:CHCOR1, which were obtained from the reaction of 3-perfluoroacylprop-2-enylidenetriphenylphosphoranes Ph3P:CHCH:CHCOR1 with Me perfluoroalkynoates R2C.tplbond.CCO2Me.

IT **34060-79-2P 150712-97-3P 150712-98-4P 150712-99-5P 150713-00-1P 150713-01-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

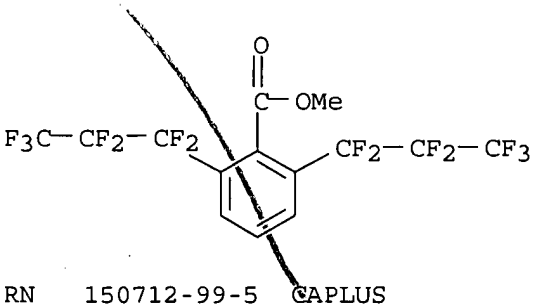
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



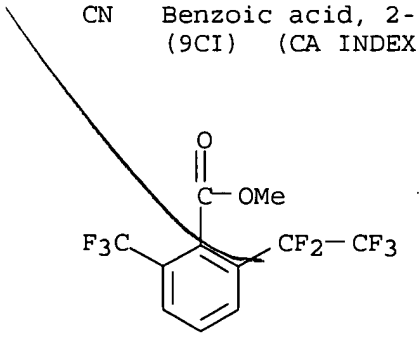
RN 150712-97-3 CAPLUS
CN Benzoic acid, 2,6-bis(pentafluoroethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 150712-98-4 CAPLUS
CN Benzoic acid, 2,6-bis(heptafluoropropyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 150712-99-5 CAPLUS
CN Benzoic acid, 2-(pentafluoroethyl)-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



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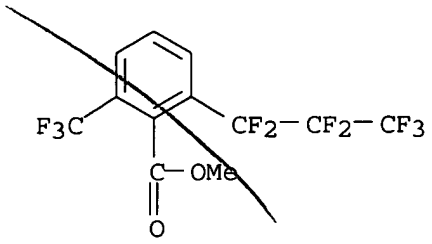
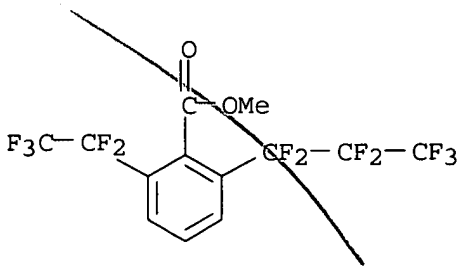
RN 150713-00-1 CAPLUS
CN Benzoic acid, 2-(heptafluoropropyl)-6-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 150713-01-2 CAPLUS
CN Benzoic acid, 2-(heptafluoropropyl)-6-(pentafluoroethyl)-, methyl ester (9CI) (CA INDEX NAME)

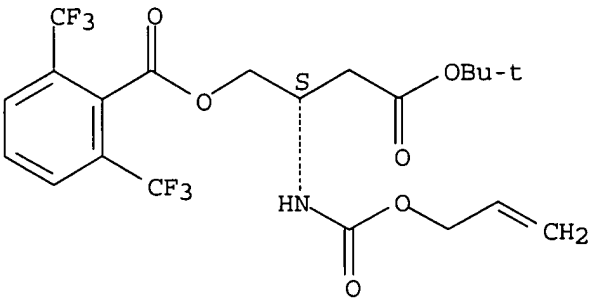


L3 ANSWER 89 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:641381 CAPLUS
DN 119:241381
TI Peptidyl derivatives as inhibitors of interleukin-1β converting enzyme
IN Chapman, Kevin T.; Maccoss, Malcolm; Mjalli, Adnan
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

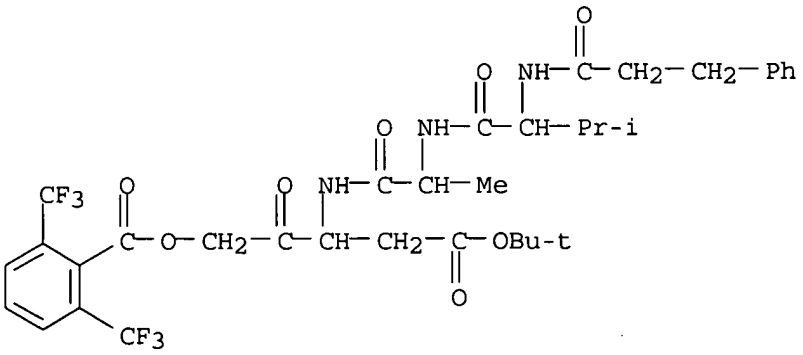
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9316710	A1	19930902	WO 1993-US1321	19930212
	W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
	AU 9336668	A1	19930913	AU 1993-36668	19930212
	EP 627926	A1	19941214	EP 1993-905939	19930212
	EP 627926	B1	19980805		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 07504194	T2	19950511	JP 1993-514912	19930212
	JP 3386125	B2	20030317		
	AT 169224	E	19980815	AT 1993-905939	19930212
	ES 2118940	T3	19981001	ES 1993-905939	19930212
	CA 2129976	C	20020917	CA 1993-2129976	19930212
	US 5430128	A	19950704	US 1994-342991	19941121
PRAI	US 1992-839590	A	19920221		
	WO 1993-US1321	A	19930212		

US 1993-67412 B1 19930525
OS MARPAT 119:241381
AB Peptidyl derivs. are provided for treatment of interleukin-1-mediated disorders or diseases. The peptide derivs. inhibit interleukin-1β converting enzyme (no data) and are useful in the treatment of inflammatory or immune-based diseases of the lungs, etc. (no data). Three compds. were prepared
IT **151272-23-0P 151272-24-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of peptide derivative for treatment of
interleukin-1-mediated diseases)
RN 151272-23-0 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 4-(1,1-dimethylethoxy)-4-oxo-2-[[(2-propenyloxy)carbonyl]amino]butyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 151272-24-1 CAPLUS
CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-[2-(1,1-dimethylethoxy)-2-oxoethyl]-2-oxopropyl]-, (S)- (9CI) (CA INDEX NAME)



IT **151272-16-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and interleukin-1-mediated diseases treatment with, interleukin-1β converting enzyme inhibition in relation to)
RN 151272-16-1 CAPLUS
CN L-Alaninamide, N-(1-oxo-3-phenylpropyl)-L-valyl-N-[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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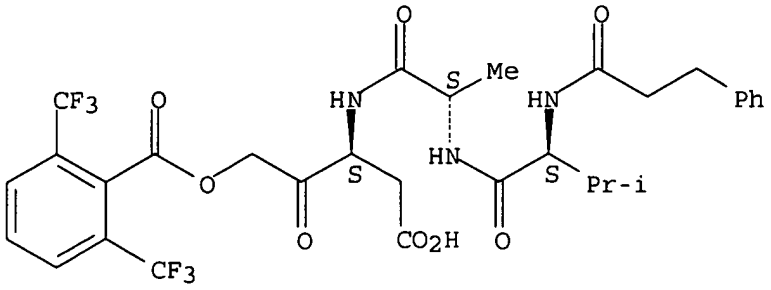
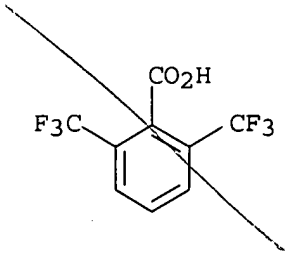


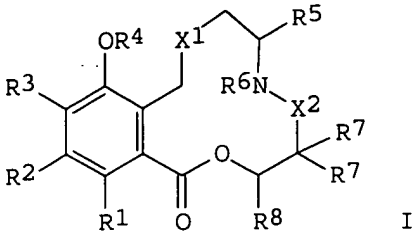
IT **24821-22-5**, 2,6-Bistrifluoromethylbenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of peptide derivative for treatment of interleukin-1-mediated diseases)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 90 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:517285 CAPLUS
DN 119:117285
TI Preparation of benzoxathiaazabicyclododecines as novel DNA gyrase inhibitors
IN Arisawa, Mikio; Goetschi, Erwin; Kamiyama, Tsutomu; Masciadri, Raffaello; Shimada, Hisao; Watanabe, Junko; Hebeisen, Paul; Link, Helmut
PA Hoffmann-La Roche, F., und Co. A.-G., Switz.
SO PCT Int. Appl., 164 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9218490	A1	19921029	WO 1992-EP809	19920409
	W: JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	EP 535192	A1	19930407	EP 1992-908147	19920409
	EP 535192	B1	19960619		
	R: AT, BE, CH, DE, DK, FR, GB, IT, LI, NL				
	JP 05508167	T2	19931118	JP 1992-507648	19920409
	AT 139532	E	19960715	AT 1992-908147	19920409
	US 5294609	A	19940315	US 1992-952537	19921209
	US 5399741	A	19950321	US 1994-177483	19940106
	US 5486466	A	19960123	US 1994-339442	19941114
PRAI	EP 1991-106105	A	19910417		
	WO 1992-EP809	W	19920409		
	US 1992-952537	A3	19921209		
	US 1994-177483	A3	19940106		

OS MARPAT 119:117285
GI



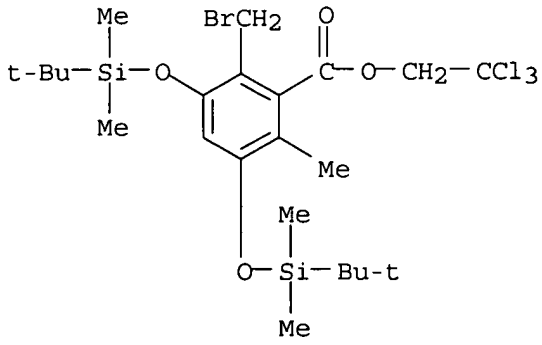
I

AB A process for the preparation of the title compds. I (X1 = S or SO, X2 = C(O) or C(S), R1 = H, alkyl, halogen, R2,R3 = H, alkyl, halogen, amino, acylamino, R4 = H, R5 = H, esterified carboxy or amidated carboxy, R6,R7 = H, alkyl, R8 = H, alkyl, esterified carboxy or amidated (thio)carboxy group) useful as antimicrobials, are prepared E.g., 1.1 g of 3,5-diacetoxy-6-[(R)-2-((S)-2-(1-tert-butoyformamido)-3-methylbenzoic acid was added to dithiobis(4-tertbutyl-1-isopropylimidazole) and PPH3 (.74 g) to give tert-Bu (4R, 7S)-12,14-diacetoxy-1,3,4,5,6,7,8,10-octahydro-4-methoxy carbonyl-11-methyl-6,10-dioxo-9,2,5-benzoxa thiaazacyclododecine-7-carbamate as white crystals.

IT **147214-78-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with (trityloxypropionylamino)mercaptopropionate)

RN 147214-78-6 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)



IT **147214-48-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with [(butoxycarbonyl)seryl]cysteine Me ester)

RN 147214-48-0 CAPLUS

CN Benzoic acid, 3,5-bis(acetyloxy)-2-(bromomethyl)-6-methyl-, chloromethyl ester (9CI) (CA INDEX NAME)

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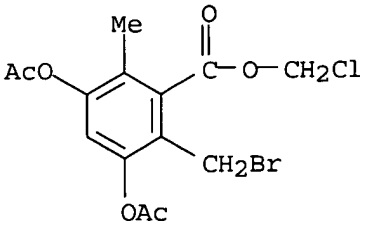
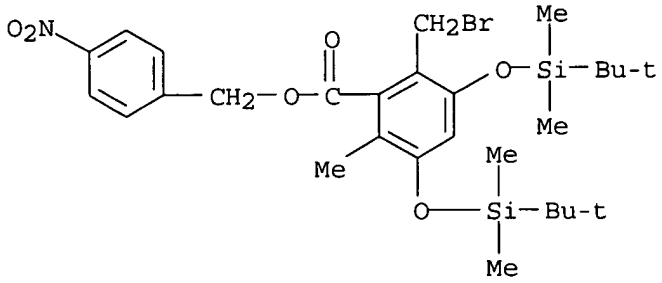
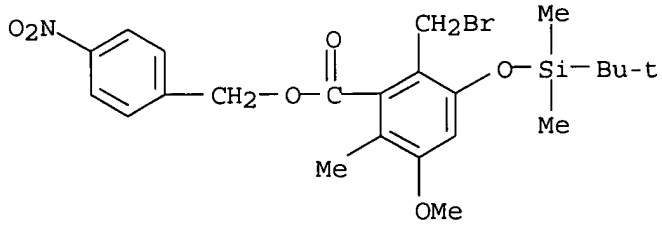


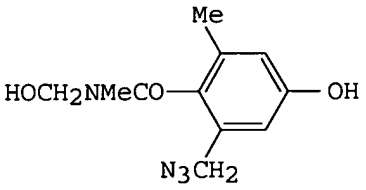
IT **147214-70-8P 147215-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with [(tert-butoxycarbonyl)seryl]cysteine Me ester)
RN 147214-70-8 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



RN 147215-10-9 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-methoxy-6-methyl-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 91 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:496144 CAPLUS
DN 119:96144
TI Synthesis of protected peptide fragments and release from a solid support under neutral conditions
AU Osborn, Nigel J.; Robinson, John A.
CS Inst. Org. Chem., Univ. Zurich, Zurich, CH-8057, Switz.
SO Tetrahedron (1993), 49(14), 2873-84
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



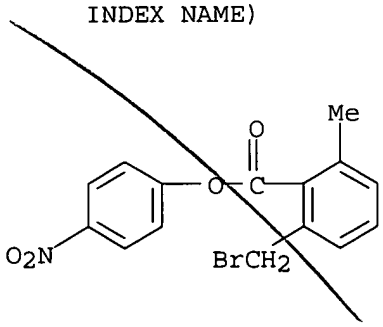
I

AB (Azidomethyl)benzamide linker I has been developed for use in solid-phase peptide synthesis which allows a protected peptide to be cleaved from the resin under neutral conditions (Bu3P, DMF, imidazole buffer pH 7) while retaining tert-butoxy, tert-butoxycarbonyl (Boc), and 9-fluorenylmethoxycarbonyl (Fmoc) protecting groups. Linker I is coupled to a polystyrene resin as a phenol ether and to the peptide via an N-hydroxymethyl ester. The protected peptide fragments so produced may be useful, for example, in subsequent fragment condensations using the Fmoc chemical

IT **149228-89-7P**, 4-Nitrophenyl 2-bromomethyl-6-methylbenzoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution of, with azide)

RN 149228-89-7 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 92 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1993:490285 CAPLUS
DN 119:90285
TI Trifluoromethylbenzene derivatives for fluorine-19 NMR imaging
IN White, David H.; Woulfe, Steven R.; Lin, Youlin; Kneller, Mills T.
PA Mallinckrodt Medical, Inc., USA
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9307907	A1	19930429	WO 1992-US9067	19921021
	W: AU, CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
	US 5318770	A	19940607	US 1991-782153	19911025
	AU 9229046	A1	19930521	AU 1992-29046	19921021
PRAI	US 1991-782153	A	19911025		
	WO 1992-US9067	A	19921021		

OS MARPAT 119:90285
GI

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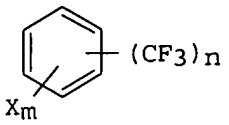


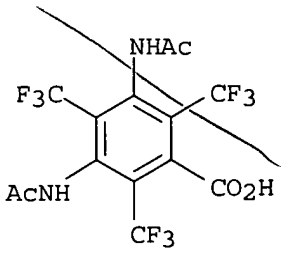
I

AB Trifluoromethylbenzene analogs (I; X = CONR1R2, NR1COR2, SO2NR1R2, CO2H; R1, R2 = H, alkyl, hydroxyalkyl; n = 1-5; m = 6 - n) of iodinated x-ray contrast media are prepared for use, alone or combined with paramagnetic substances, in 19F NMR imaging. Thus, 3,5-bis(trifluoromethyl)benzoyl chloride is condensed with 3-amino-1,2-propanediol to provide N-(2,3-dihydroxypropyl)-3,5-bis(trifluoromethyl)benzenecarboxamide (no data).

IT **149206-72-4**
RL: BIOL (Biological study)
(as NMR imaging contrast agent)

RN 149206-72-4 CAPLUS

CN Benzoic acid, 3,5-bis(acetylamino)-2,4,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 93 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:427890 CAPLUS

DN 119:27890

TI Synthesis and characterization of "picnic-basket" porphyrins with a substituent in the interior of the pocket

AU Michida, Takashi; Kyuhara, Masahiro; Nishiyama, Michiko; Yoshimi, Yukihiro; Fitzgerald, Jeffrey P.; Sayo, Hiroteru

CS Fac. Pharm. Sci., Kobe-Gakuin Univ., Kobe, 651-21, Japan

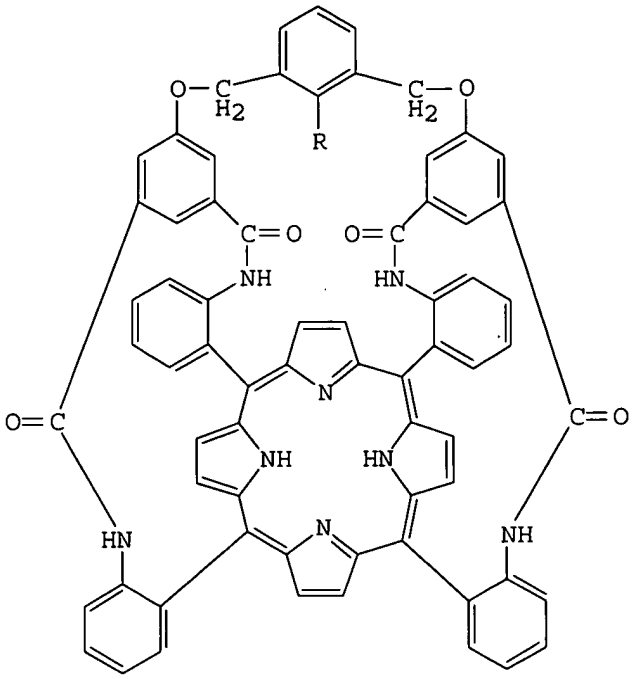
SO Chemical & Pharmaceutical Bulletin (1992), 40(12), 3157-62
CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

GI

10803578



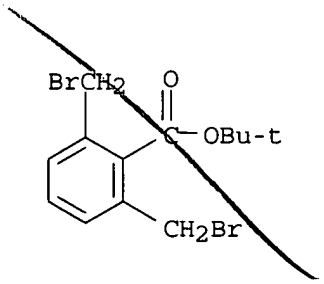
I

AB The title compds. I (R = H, CO2Et, CO2H, CONH2) were synthesized to study stabilization of the bound oxygen in hemoprotein models. The Co(II) complexes of I have enormous equilibrium consts. for the formation of base adducts, while H-bonding interaction with coordinated dioxygen is not as effective for stabilization of the metal-dioxygen bond as was expected. The results suggest that doming of the porphyrin plane plays an important role in the binding of dioxygen.

IT **56263-53-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution of, with hydroxyisophthalate)

RN 56263-53-7 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 94 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:54913 CAPLUS

DN 118:54913

TI Comparative behavior of calpain and cathepsin B toward peptidyl acyloxymethyl ketones, sulfonium methyl ketones and other potential inhibitors of cysteine proteinases

AU Pliura, Diana H.; Bonaventura, Bonnie J.; Smith, Roger A.; Coles, Peter J.; Krantz, Allen

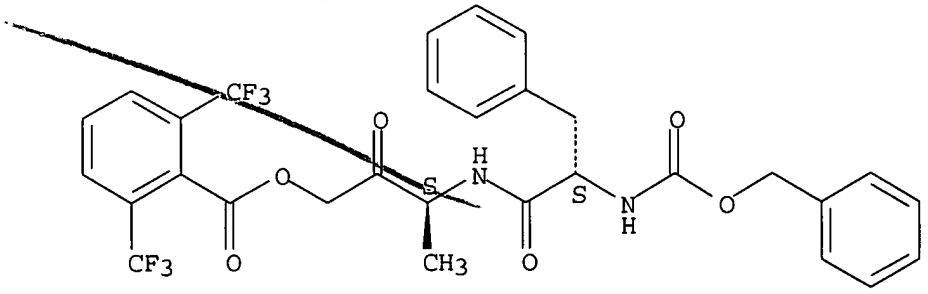
CS Syntex Res., Mississauga, ON, L5N 3X4, Can.

SO Biochemical Journal (1992), 288(3), 759-62
CODEN: BIJOAK; ISSN: 0306-3275

10803578

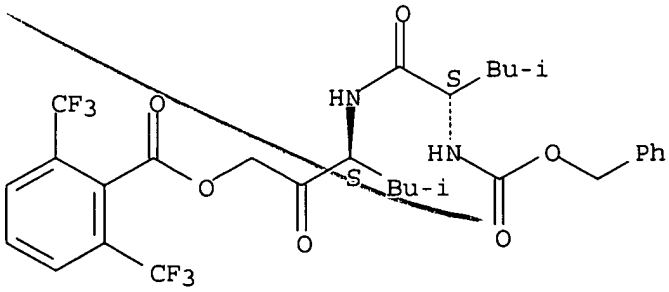
DT Journal
LA English
AB Peptidyl acyloxymethyl ketones, previously established as potent inactivators of the lysosomal cysteine proteinase cathepsin B, were evaluated against smooth-muscle calpain, a member of the family of Ca2+-dependent cysteine proteinases. Only modest rates of time-dependent inhibition could be achieved, even with peptidyl affinity groups optimized for calpain and linked to a carboxylate leaving group of very low pKa [2,6-(CF3)2PhCOO-, pKa 0.58]. Selective inactivation of cathepsin B vs. calpain was consistently observed with this type of inhibitor. Examination of other potential inhibitors revealed a rank order of potency against calpain to be: peptidyl sulfonium Me ketones > fluoromethyl ketones, diazomethyl ketones » acyloxymethyl ketones, an order which differs sharply from that found for cathespin B.
IT **115186-03-3**
RL: BIOL (Biological study)
(calpain and cathepsin B inhibition by, kinetics of, structure in relation to)
RN 115186-03-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



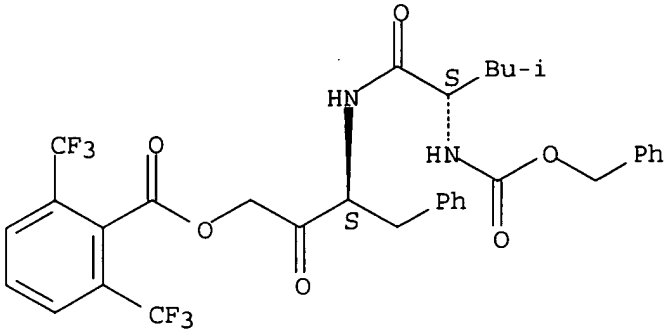
IT **118252-88-3P 118252-89-4P 145428-00-8P 145428-01-9P 145428-02-0P 145482-29-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and calpain and cathepsin B inhibition and kinetics by, structure in relation to)
RN 118252-88-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 5-methyl-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-2-oxohexyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



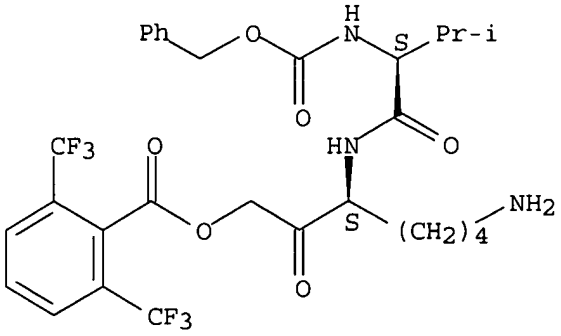
RN 118252-89-4 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-2-oxo-4-phenylbutyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



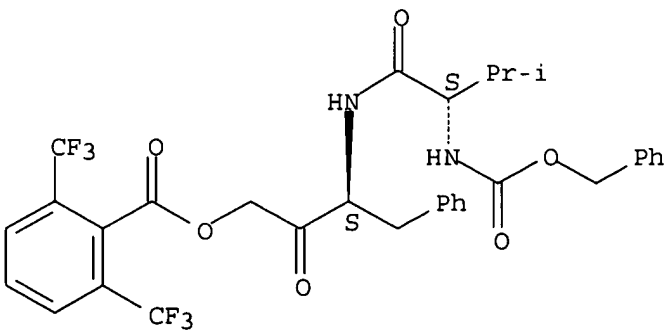
RN 145428-00-8 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 7-amino-3-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-2-oxoheptyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

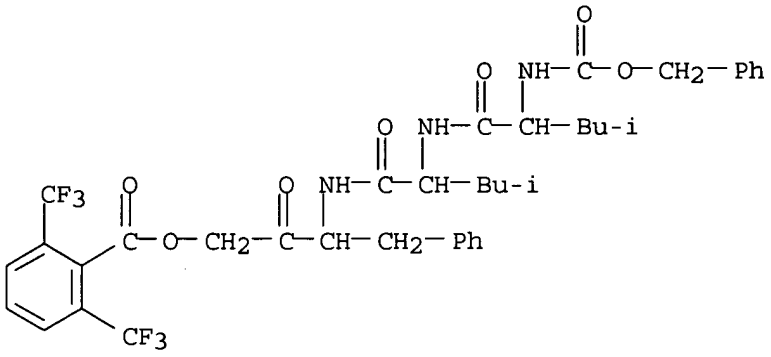


RN 145428-01-9 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 3-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-2-oxo-4-phenylbutyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

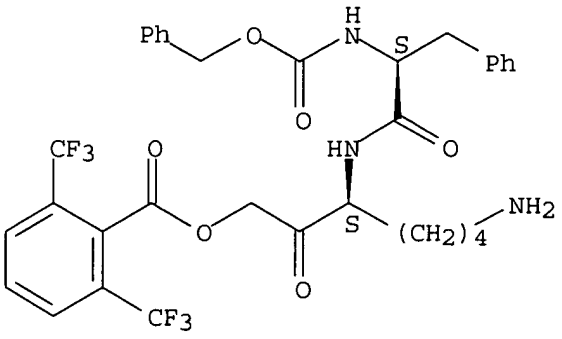


RN 145428-02-0 CAPLUS
CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-2-oxo-1-(phenylmethyl)propyl]-, (S)- (9CI) (CA INDEX NAME)



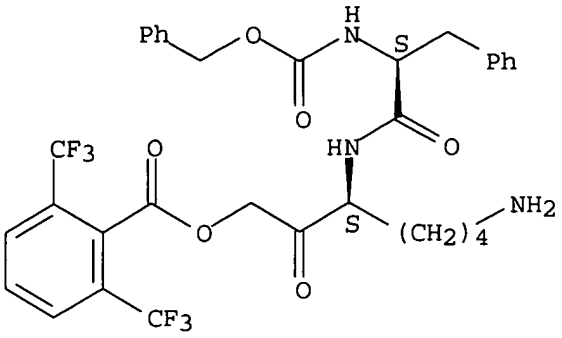
RN 145482-29-7 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 7-amino-2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]heptyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **133524-91-1P 145428-05-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 133524-91-1 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 7-amino-2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]heptyl ester, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

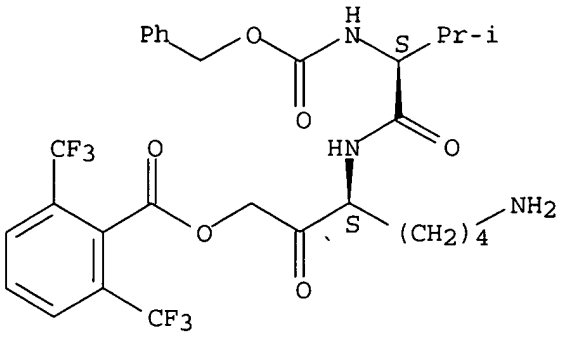
Absolute stereochemistry.



● HCl

RN 145428-05-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 7-amino-3-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-2-oxoheptyl ester, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L3 ANSWER 95 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:634646 CAPLUS
DN 117:234646
TI Para-linked aromatic poly(amic ethyl esters): precursors to rodlike aromatic polyimides. 1. Synthesis and imidization study
AU Becker, Kevin H.; Schmidt, Hans Werner
CS Mater. Dep., Univ. California, Santa Barbara, CA, 93106, USA
SO Macromolecules (1992), 25(25), 6784-90
CODEN: MAMOBX; ISSN: 0024-9297
DT Journal
LA English
AB The synthesis and characterization of several para-linked aromatic poly(amic Et esters) are described. These substituted polyamides are precursors to rodlike aromatic polyimides. The poly(amic Et esters) are prepared from 2,5-bis(ethoxycarbonyl)terephthaloyl chloride and several substituted 1,4-diaminobenzene and noncoplanar 4,4'-diaminobiphenylene derivs. Depending on the degree and type of substitution, the precursors are soluble

to high concns. in solvents such as DMF or N-methylpyrrolidinone without the addition of inorg. salts. In addition to the characterization of the precursor polyamides, a detailed chemical and thermal study of the imidization process is presented, based on dynamic and isothermal TGA measurements and FT-IR spectroscopy investigations.

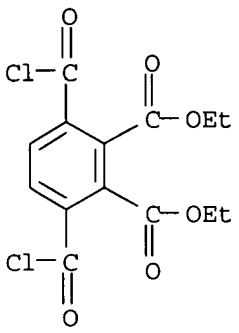
IT **143969-54-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in presence of chlorotrimethylsilane)

RN 143969-54-4 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3,6-bis(chlorocarbonyl)-, diethyl ester, polymer with [1,1'-biphenyl]-2,5-diamine and diethyl 2,5-bis(chlorocarbonyl)-1,4-benzenedicarboxylate (9CI) (CA INDEX NAME)

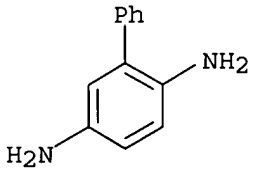
CM 1

CRN 143969-53-3
CMF C14 H12 Cl2 O6



CM 2

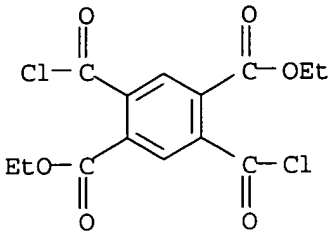
CRN 109942-17-8
CMF C12 H12 N2



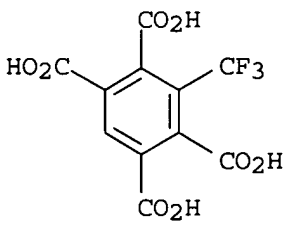
CM 3

CRN 6423-33-2
CMF C14 H12 Cl2 O6

10803578

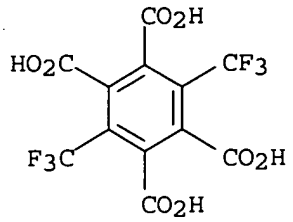


L3 ANSWER 96 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:490923 CAPLUS
DN 117:90923
TI Polyimides derived from 2,2'-bis(trifluoromethyl)-4,4'-diaminobiphenyl. 2. Synthesis and characterization of polyimides prepared from fluorinated benzenetetracarboxylic dianhydrides
AU Matsuura, Tohru; Ishizawa, Maki; Hasuda, Yoshinori; Nishi, Shiro
CS Interdisc. Res. Lab., NTT, Tokyo, 180, Japan
SO Macromolecules (1992), 25(13), 3540-5
CODEN: MAMOBX; ISSN: 0024-9297
DT Journal
LA English
AB Fluorinated rigid-rod polyimides are prepared by the polymerization of 2,2'-bis(trifluoromethyl)-4,4'-diaminobiphenyl (I) with 1,4-bis(trifluoromethyl)-2,3,5,6-benzenetetracarboxylic dianhydride (II), 1-(trifluoromethyl)-2,3,5,6-benzenetetracarboxylic dianhydride, or pyromellitic dianhydride (III). The dielec. constant, refractive index, and water absorption of the copolymers decrease with an increasing number of CF3 side chains. The I-II polyimide, which has the highest F content, has the lowest dielec. constant of 2.6 at 1 MHz, the lowest refractive index of 1.490 at 589.3 nm, and the lowest water absorption of 0.38%. The coefficient of thermal expansion (CTE) of the copolymers increases with an increasing number of CF3 side chains. I-III polyimide has a neg. CTE of -5 + 10-6 °C-1 by thermomech. anal. and a high polymer decomposition temperature of 613° measured for a 10% weight loss in a N atmospheric by TG.
IT **53812-59-2P 128298-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acid anhydride conversion of)
RN 53812-59-2 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 128298-23-7 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 97 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:469858 CAPLUS
DN 117:69858
TI Preparation of 2-saccharinylmethyl benzoates and related compounds as protease inhibitors
IN Dunlap, Richard Paul; Boaz, Neil Warren; Mura, Albert Joseph; Subramanyam, Chakrapani; Kumar, Virendra; Desai, Ranjit Chimanlal; Hlasta, Dennis John; Saindane, Manohar Tukram; Bell, Malcolm Rice; Court, John Joseph
PA Sterling Winthrop Inc., USA
SO Eur. Pat. Appl., 84 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 7

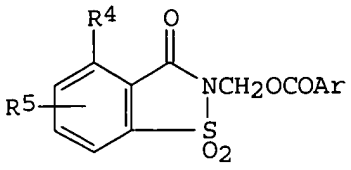
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 483928	A1	19920506	EP 1991-202809	19911030
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AU 9186083	A1	19920507	AU 1991-86083	19911024
	AU 642537	B2	19931021		
	SG 69977	A1	20000125	SG 1996-7579	19911030
	CA 2054653	AA	19920502	CA 1991-2054653	19911031
	HU 63399	A2	19930830	HU 1991-3430	19911031
	IL 99913	A1	19961114	IL 1991-99913	19911031
	IL 114773	A1	19961205	IL 1991-114773	19911031
	FI 9105163	A	19920502	FI 1991-5163	19911101
	FI 103112	B1	19990430		
	NO 9104288	A	19920504	NO 1991-4288	19911101
	NO 300373	B1	19970520		
	JP 04273866	A2	19920930	JP 1991-288080	19911101
	RU 2114843	C1	19980710	RU 1991-5010338	19911101
	NO 9202976	A	19920504	NO 1992-2976	19920728
	NO 301116	B1	19970915		
	US 5380737	A	19950110	US 1993-113508	19930827
	HU 70756	A2	19951030	HU 1994-569	19940225
	HU 70764	A2	19951030	HU 1994-580	19940225
	US 5464852	A	19951107	US 1994-289113	19940811
	FI 9404968	A	19941021	FI 1994-4968	19941021
	US 5578623	A	19961126	US 1995-445240	19950519
	FI 9600490	A	19960202	FI 1996-490	19960202
	FI 103115	B1	19990430		
	US 5773456	A	19980630	US 1996-719216	19960925
PRAI	US 1990-608068	A	19901101		
	US 1989-347125	B2	19890504		
	US 1989-347126	B2	19890504		
	US 1990-514920	A	19900426		
	US 1991-782016	A	19911024		
	HU 1991-3430	A	19911031		
	IL 1991-99913	A3	19911031		
	FI 1991-5163	A	19911101		

10803578

	NO 1991-4288	A1	19911101
	US 1991-793035	B1	19911115
	US 1993-113508	A3	19930827
	US 1994-289113	A3	19940811
	FI 1994-4968	A	19941021
	US 1995-445240	A3	19950519

OS MARPAT 117:69858

GI



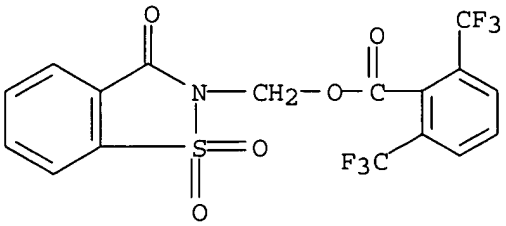
I

AB Title compds. I [Ar = substituted Ph, -naphthyl, -anthryl; R4 = H, halo, C1-10 alkyl, C1-10 perfluoroalkyl, C1-10 perchloroalkyl, C2-10 alkenyl, C2-10 alkynyl, cyano, (substituted) amino, C1-10 alkoxy, PhCH2O, C2-11 alkoxycarbonyl, Ph, CONH2; R5 = H, halo, cyano, NO2, (substituted) amino, C1-10 alkylsulfonylamino, SO2NH2, (substituted) C1-10 alkyl, cycloalkyl, C1-10 alkoxy, OH, CO2H, CHO, CH2NH2, etc.; or R5 5- or 6-membered fused saturated heterocyclyl containing 2 atoms selected from N, O, S; with provisos] were prepared as protease inhibitors useful for the treatment of degenerative diseases. Thus, a mixture of 2-chloromethyl-4,6-dimethoxysaccharin (preparation given), 2,6-dichlorobenzoic acid, and Et3N in PhMe was refluxed for 6 h to give 4,6-dimethoxy-2-saccharinylmethyl 2,6-dichlorobenzoate (II). II had Ki of 0.08 nM vs. protease.

IT **142426-83-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as protease inhibitor)

RN 142426-83-3 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl)methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 98 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:130739 CAPLUS

DN 116:130739

TI Amorphous polymers for optical transmitting systems and optical members and their use

IN Takezawa, Yoshitaka; Ohara, Shuichi; Tanno, Seikich; Taketani, Noriaki; Shimura, Masato

PA Hitachi, Ltd., Japan

SO Eur. Pat. Appl., 31 pp.
CODEN: EPXXDW

DT Patent

10803578

LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 454165	A2	19911030	EP 1991-106851	19910426
	EP 454165	A3	19930120		
	R: DE, FR, GB, IT, NL				
	JP 04009805	A2	19920114	JP 1990-112511	19900427
	JP 2854669	B2	19990203		
	US 5093888	A	19920303	US 1991-686997	19910418
PRAI	JP 1990-112511	A	19900427		

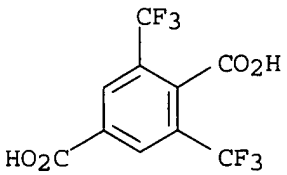
AB The title polymers, e.g., polyether-polyketones, polyarylates, polyimides, and polyesters, have good heat resistance and low attenuation and are useful as optical transmitting systems, e.g., for controlling ignition timing and fuel metering systems for internal combustion engines in automobiles. Thus, an optical fiber comprised a core of amorphous PEEK and a sheath of poly(2,2,2-trifluoroethyl methacrylate).

IT **138704-67-3 138704-69-5 138761-84-9**
RL: USES (Uses)
(optical fibers, heat-resistant, for engine control systems)

RN 138704-67-3 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,6-bis(trifluoromethyl)-, polymer with 2,2'-oxybis[ethanol] (9CI) (CA INDEX NAME)

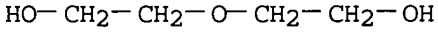
CM 1

CRN 138704-66-2
CMF C10 H4 F6 O4



CM 2

CRN 111-46-6
CMF C4 H10 O3

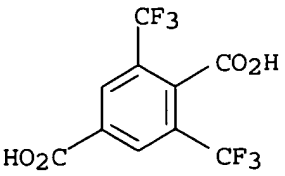


RN 138704-69-5 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,6-bis(trifluoromethyl)-, polymer with 1,2-ethanediol (9CI) (CA INDEX NAME)

CM 1

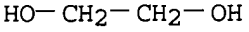
CRN 138704-66-2
CMF C10 H4 F6 O4

10803578



CM 2

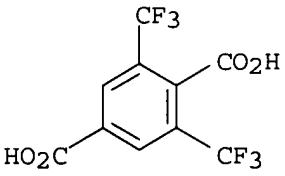
CRN 107-21-1
CMF C2 H6 O2



RN 138761-84-9 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,6-bis(trifluoromethyl)-, polymer with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (9CI) (CA INDEX NAME)

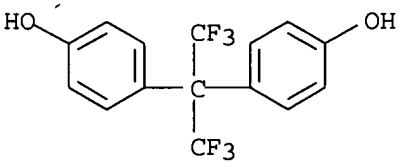
CM 1

CRN 138704-66-2
CMF C10 H4 F6 O4



CM 2

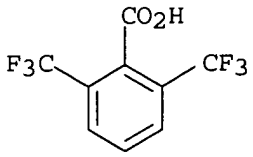
CRN 1478-61-1
CMF C15 H10 F6 O2



L3 ANSWER 99 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:125114 CAPLUS
DN 116:125114
TI Specificity of pyridinemonocarboxylates and benzoic acid analogs as chemical hybridizing agents in wheat
AU Ciha, Allan J.; Ruminski, Peter G.
CS Monsanto Agric. Co., St. Louis, MO, 63167, USA
SO Journal of Agricultural and Food Chemistry (1991), 39(11), 2072-6

10803578

CODEN: JAFCAU; ISSN: 0021-8561
DT Journal
LA English
AB A series of substituted pyridinemonocarboxylates and benzoic acids were evaluated in growth chambers as potential chemical hybridizing agents for wheat (Triticum aestivum). Chemical hybridizing potential, measured as spike sterility, was observed with both areas of chemical The 3-pyridinecarboxylic acid, 4-hydroxy-2,6-bis(trifluoromethyl) Me ester, and 2,4-bis(trifluoromethyl)benzoic acid were the only mols. to exhibit complete spike sterility. Minor changes in both mols. resulted in total loss of activity. Substitutions at the 4-position on the pyridinemonocarboxylate which are subject to hydrolysis to the 4-hydroxyl or which contained an acidic proton functionality were the only substitutions exhibiting any level of spike sterility.
IT **24821-22-5**
RL: BIOL (Biological study)
(wheat spike stability induction by, hybridizing potentials in relation to)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



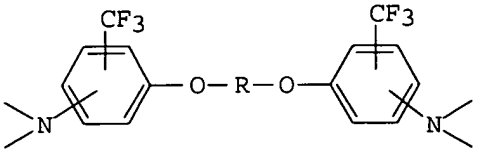
L3 ANSWER 100 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:95927 CAPLUS
DN 116:95927
TI Liquid-crystal display device containing polyimide orientation films
IN Hanyu, Yukio
PA Canon K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 03006528	A2	19910114	JP 1989-141395	19890602
	JP 2556589	B2	19961120		
	US 5192596	A	19930309	US 1990-529509	19900529
	EP 400635	A2	19901205	EP 1990-110314	19900530
	EP 400635	A3	19910320		
	EP 400635	B1	19950927		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 128561	E	19951015	AT 1990-110314	19900530
	ES 2076990	T3	19951116	ES 1990-110314	19900530
	US 5316805	A	19940531	US 1992-981432	19921125
	US 5426525	A	19950620	US 1993-55357	19930503
PRAI	JP 1987-234357	A	19870917		
	JP 1987-232502	A	19870918		
	JP 1988-225049	A	19880907		
	US 1988-245644	A3	19880916		
	JP 1989-141395	A	19890602		
	JP 1989-141396	A	19890602		
	JP 1989-160278	A	19890622		

10803578

US 1990-495607	A3	19900319
JP 1990-109658	A	19900424
US 1990-529509	A3	19900529
US 1992-981432	A	19921125
US 1992-998817	A	19921230

GI



I

AB The title device has a pair of substrates, a polyimide film containing a structure unit I (R = arylene) on at least 1 of the substrates, and ferroelec. liquid crystals between the substrates.

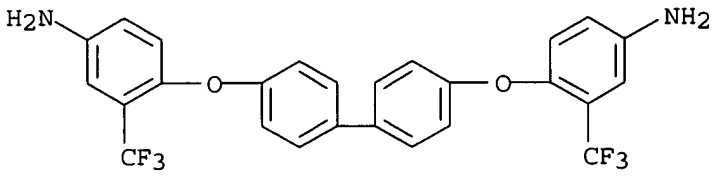
IT **138322-00-6 138322-03-9**
RL: USES (Uses)
(liquid-crystal display devices containing orientation films of)

RN 138322-00-6 CAPLUS

CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(trifluoromethyl)-, polymer with 4,4'-[[1,1'-biphenyl]-4,4'-diylbis(oxy)]bis[3-(trifluoromethyl)benzenamine] (9CI) (CA INDEX NAME)

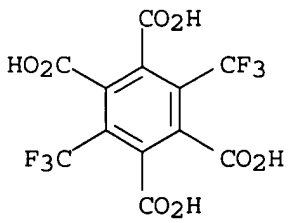
CM 1

CRN 138321-99-0
CMF C26 H18 F6 N2 O2



CM 2

CRN 128298-23-7
CMF C12 H4 F6 O8



RN 138322-03-9 CAPLUS

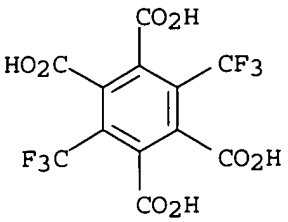
CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(trifluoromethyl)-, polymer with 4,4'-[1,4-phenylenebis(oxy)]bis[3-(trifluoromethyl)benzenamine] (9CI)

10803578

(CA INDEX NAME)

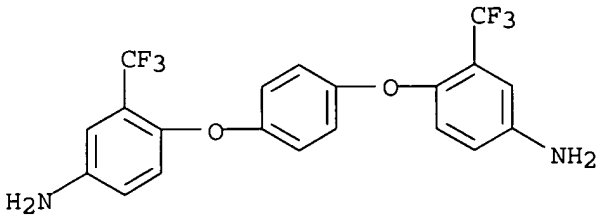
CM 1

CRN 128298-23-7
CMF C12 H4 F6 O8



CM 2

CRN 94525-05-0
CMF C20 H14 F6 N2 O2



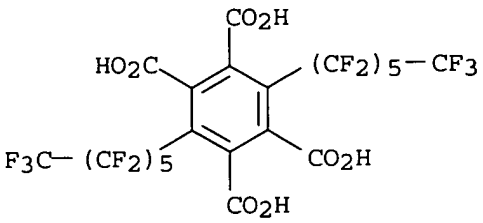
L3 ANSWER 101 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:42560 CAPLUS
DN 116:42560
TI Fluorine-containing polyamic acids and polyimides
IN Yamamoto, Michiharu; Nishikimi, Tadashi
PA Nitto Denko Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 03221524	A2	19910930	JP 1990-16491	19900126
PRAI JP 1990-16491		19900126		

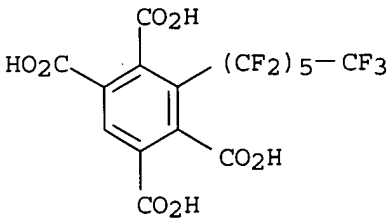
AB Polyamic acids and polyimides are prepared from 3-(perfluoroalkyl)- or 3,6-bis(perfluoroalkyl)pyromellitic acid or derivs. Thus, polymerization of 3-(perfluorohexyl)pyromellitic anhydride with 4,4'-(hexafluoroisopropylidene)dianiline and cyclization gave a polyimide film with dielec. constant 2.50 and moisture absorption 0.19%.
IT **138522-77-7P 138522-79-9P**
RL: PREP (Preparation)
(preparation of)
RN 138522-77-7 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(tridecafluorohexyl)- (9CI)

10803578

(CA INDEX NAME)



RN 138522-79-9 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

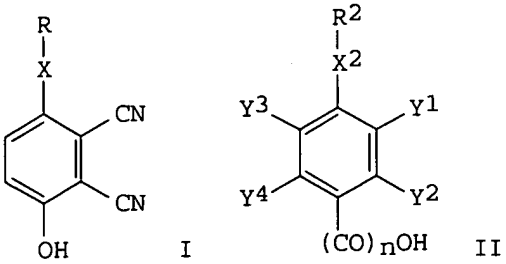


L3 ANSWER 102 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:13515 CAPLUS
DN 116:13515
TI Liquid crystal composition, liquid crystal device, display apparatus and display method using same
IN Yoshida, Akio; Togano, Takeshi; Sato, Junko
PA Canon K. K., Japan
SO Eur. Pat. Appl., 89 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

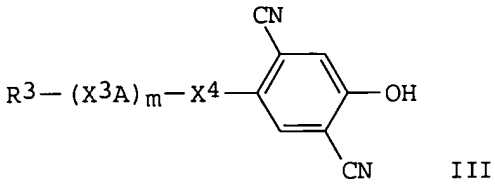
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 442499	A2	19910821	EP 1991-102104	19910214
	EP 442499	A3	19920805		
	EP 442499	B1	19950920		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 04211492	A2	19920803	JP 1991-11000	19910131
	JP 3143483	B2	20010307		
	US 5217643	A	19930608	US 1991-653233	19910211
	AT 128172	E	19951015	AT 1991-102104	19910214
PRAI	JP 1990-35233	A	19900215		
	JP 1990-35234	A	19900215		
	JP 1990-35235	A	19900215		
	JP 1991-11000	A	19910131		

OS MARPAT 116:13515
GI

10803578



I II



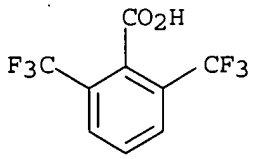
III

AB A liquid crystal composition is described comprising ≥1 compound from I, II, and III [R, R2 = H, alkyl, R1-p-C6H10 (when X = CO2 or CH2O); R1 = alkyl, alkoxy; R3 = alkyl; X = O, CO2, O2C, CH2O (only when R = R1-p-C6H10); X2, X3 = O, CO2, O2C; X4 = O, CO2, CH2O; Y1-Y4 = H, F, CF3; ≥1 of Y1-Y4 = F, CF3; A = p-C6H4, p-C6H10; m, n = 0, 1]. A display device containing the above composition and a display method using the device are also claimed. The composition has a specific resistivity modifier, improving display characteristics.

IT **24821-22-5**
RL: USES (Uses)
(resistivity modifier, in liquid crystal composition)

RN 24821-22-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 103 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:679936 CAPLUS

DN 115:279936

TI Studies on antiatherosclerotic agents. Synthesis and inhibitory activities on platelet aggregation of 4-aryl derivatives of 7-ethoxycarbonyl-6,8-dimethyl-1(2H)-phthalazinone

AU Eguchi, Yukuo; Sato, Yuko; Sekizaki, Satomi; Ishikawa, Masayuki

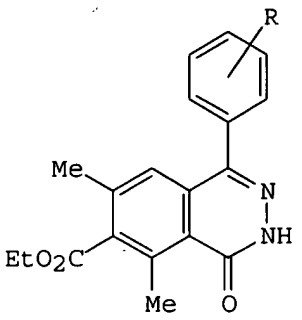
CS Inst. Med. Dent. Eng., Tokyo Med. Dent. Univ., Tokyo, 101, Japan

SO Chemical & Pharmaceutical Bulletin (1991), 39(8), 2009-15
CODEN: CPBTAL; ISSN: 0009-2363

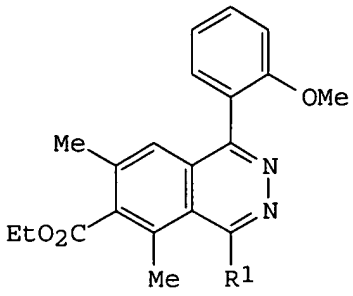
DT Journal

LA English

GI



I



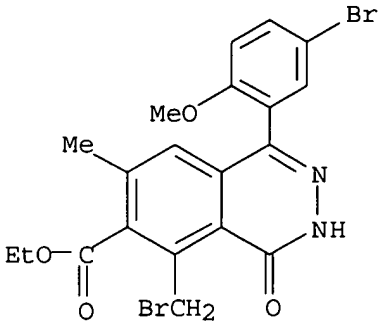
II

AB Phthalazine derivs., e.g. I (R = H, 2-, 3-, 4-Me, 2-, 4-OMe, 2-, 4-Cl, 2-, 4-OCH2Ph, etc.) and II (R1 = OEt, SEt, 1-piperidinyl, NHC6H4Cl-3, C.tplbond.CPh, etc.), were prepared and evaluated as inhibitors of arachidonic acid (AA) and ADP induced platelet aggregation. Thus, 4-ethoxycarbonyl-3,5-dimethylphthalic anhydride reacted with (RC6H4)2Cd and cyclized with H2NNH2 to give I. Some compds. had considerable inhibitory activity against AA-induced platelet aggregation. Structure activity relationships were also examined

IT **137208-02-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 137208-02-7 CAPLUS

CN 6-Phthalazinecarboxylic acid, 1-(5-bromo-2-methoxyphenyl)-5-(bromomethyl)-3,4-dihydro-7-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

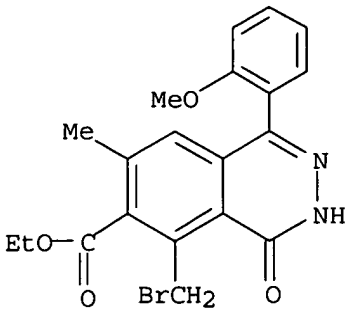


IT **137208-01-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, acetylation, and cyclocondensation of, with ammonia)

RN 137208-01-6 CAPLUS

CN 6-Phthalazinecarboxylic acid, 5-(bromomethyl)-3,4-dihydro-1-(2-methoxyphenyl)-7-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

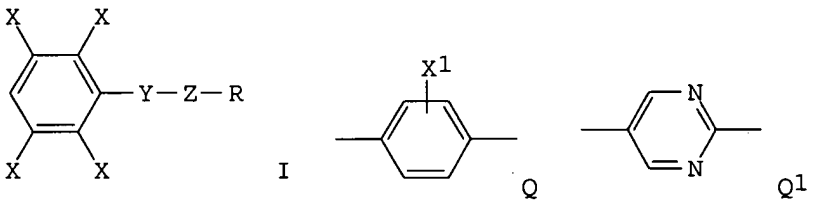
10803578



L3 ANSWER 104 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:619697 CAPLUS
DN 115:219697
TI Preparation of liquid crystal compositions
IN Mori, Yoshimasa; Takiguchi, Takao; Iwaki, Takashi; Tokano, Goji; Yamada, Yoko
PA Canon K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 31 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 02255635	A2	19901016	JP 1989-77060	19890328
PRAI JP 1989-77060		19890328		

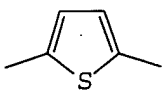
OS MARPAT 115:219697
GI



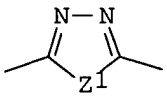
I

Q

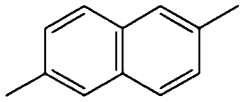
Q1



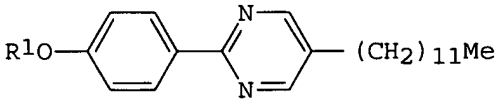
Q2



Q3



Q4

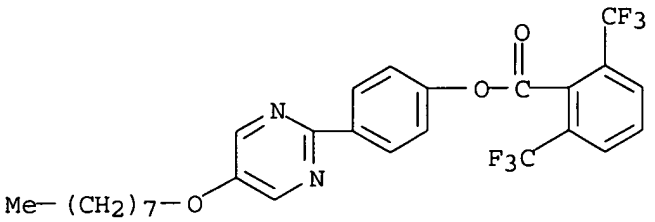


II

AB Liquid crystal compns. comprising I [R = (substituted) C1-16 alkyl, alkoxy, alkoxycarbonyl, acyloxy, alkoxycarbonyloxy; X = H, CF3, but at least one is CF3; Y = CO2, O2C, CH2O, OCH2; Z = 1,4-cyclohexylene, Q-Q4 wherein X1 = H, F, Cl, Br, cyano, Me; Z1 = O, S] are prepared A mixture of m-CF3C6H4CO2H, a phenol derivative II (R1 = H), DCC, and pyrrolidinopyridine in CH2Cl2 was stirred at room temperature to give 69% ester II (R1 = m-CF3C6H4CO), which

showed crystalline-isotropic-smectic A-smectic C transition temperature of 77.8°, 68.4°, and 62.1°, resp.

IT **132807-82-0**
RL: PRP (Properties)
(liquid crystal composition containing)
RN 132807-82-0 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 4-[5-(octyloxy)-2-pyrimidinyl]phenyl ester (9CI) (CA INDEX NAME)



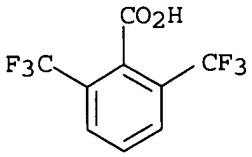
L3 ANSWER 105 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:582797 CAPLUS
DN 115:182797
TI Regioselective lithiation of 1,3-bis(trifluoromethyl)benzene with lithiated salt of secondary amine
IN Masciadri, Raffaello
PA Hoffmann-La Roche, F., A.-G., Switz.
SO Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 442340	A2	19910821	EP 1991-101437	19910204
	EP 442340	A3	19920122		
	EP 442340	B1	19950222		
	R: AT, BE, CH, DE, DK, FR, GB, IT, LI, NL				
	US 5162577	A	19921110	US 1991-649089	19910201
	CN 1054068	A	19910828	CN 1991-100927	19910212
	CN 1028994	B	19950621		
	JP 07070140	A2	19950314	JP 1991-38939	19910212
	JP 07119228	B4	19951220		
	CN 1108640	A	19950920	CN 1994-115664	19940905
PRAI	CH 1990-463	A	19900213		

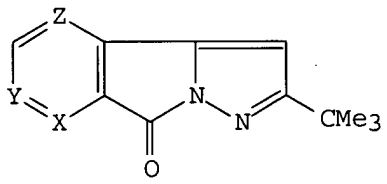
OS CASREACT 115:182797; MARPAT 115:182797
AB Regioselective lithiation of 1,3-(F3C)2C6H4 with lithium salts of secondary amines is claimed. Thus, lithiation of 1,3-(F3C)2C6H4 with the lithium salt of 2,2,6,6-tetramethylpiperidine (I), prepared in situ by the reaction of I with BuLi in THF-hexane, followed by treatment with solid CO2 and acidic workup gave 80% 2,4-(F3C)2C6H3CO2H.

IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

10803578

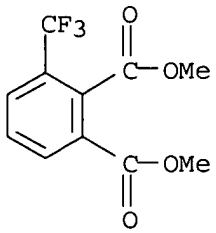


L3 ANSWER 106 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:471464 CAPLUS
DN 115:71464
TI Synthesis and structure of pyrazolo[5,1-a]isoindol-8-ones from aromatic ortho diesters
AU Chupp, John P.; Leo, Gregory C.; Molyneaux, John M.
CS Tech. Div., Monsanto Agric. Co., St. Louis, MO, 63167, USA
SO Journal of Heterocyclic Chemistry (1991), 28(3), 613-17
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
GI



I

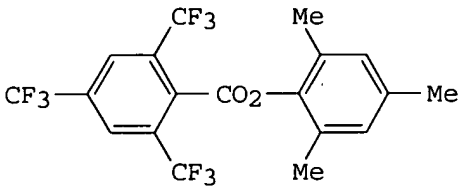
AB Title compds I (X = Z = N, Y = CH; X = Z = CH, Y= N; X = Y = CH, Z = N, CCF3; X = Y = Z = CH) were prepared by condensation of pinacolone with an appropriate diester followed by treatment with hydrazine and optionally SOCl2. Thus, di-Et 3,4-pyridinedicarboxylate so treated afforded I (X = Z = CH, Y = N).
IT **135038-85-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with pinacolone)
RN 135038-85-6 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 107 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:471045 CAPLUS
DN 115:71045
TI New aspects of the chemistry of 2,4,6-tris(trifluoromethyl)benzoic acid and related compounds
AU Filler, Robert; Gnandt, William K.; Chen, Wei; Lin, Shan

10803578

CS Dep. Chem., Illinois Inst. Technol., Chicago, IL, 60616, USA
SO Journal of Fluorine Chemistry (1991), 52(1), 99-105
CODEN: JFLCAR; ISSN: 0022-1139
DT Journal
LA English
GI

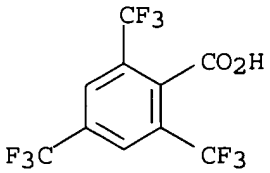


I

AB 1,3,5-Tris(trifluoromethyl)benzene reacts with BuLi and CO2 to give a high yield of 2,4,6-tri(trifluoromethyl)benzoic acid. The acid has been well characterized by spectral and pKa data. The acid chloride is formed only slowly under stringent conditions. The acid fails to undergo normal esterification with ethanol because of steric hindrance to the tetrahedral intermediate. The ester does form via the linear acylium ion. A highly substituted phenolic ester I of the acid has been obtained via s mixed anhydride with (CF3CO)2O.

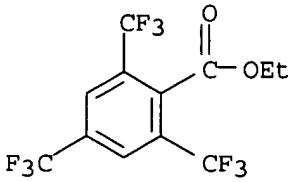
IT **25753-26-8P**, 2,4,6-Tris(trifluoromethyl)benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

RN 25753-26-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



IT **135103-71-8P 135103-72-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

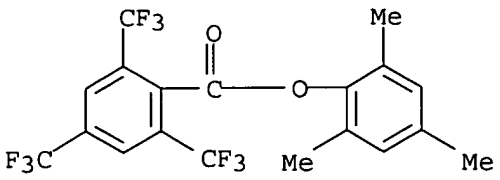
RN 135103-71-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



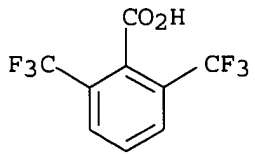
RN 135103-72-9 CAPLUS

10803578

CN Benzoic acid, 2,4,6-tris(trifluoromethyl)-, 2,4,6-trimethylphenyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 108 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:409103 CAPLUS
DN 115:9103
TI Dexamethasone 21-(β-isothiocyanatoethyl)thio ether: a new affinity label for glucocorticoid receptors
AU Lopez, Susana; Simons, S. Stoney, Jr.
CS Steroid Horm. Sect., NIDDK, Bethesda, MD, 20892, USA
SO Journal of Medicinal Chemistry (1991), 34(6), 1762-7
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 115:9103
AB The C-21 methanesulfonate ester of the synthetic glucocorticoid dexamethasone (I) is an efficient electrophilic affinity label of glucocorticoid receptors and exhibits irreversible antiglucocorticoid activity. In an effort to obtain other affinity labeling steroids with differing biol. activities, several new derivs. of I were prepared which contained a reactive electrophilic substituent at various distances from the C-21 position. All compds. displayed relatively low affinity for rat glucocorticoid receptors (≤8% of that of I) in a cell-free competition assay. Nevertheless, one compound, dexamethasone 21-(β-isothiocyanatoethyl)thio ether (II), appeared to be an affinity label by virtue of its ability to block the cell-free exchange binding of [3H]I. [3H]II was then synthesized and reacted with cell-free receptors to give, after anal. on denaturing SDS-polyacrylamide gels, only one specifically labeled species at 98 kDa, which is the mol. weight of authentic rat glucocorticoid receptor. These data directly establish II as a new affinity label for glucocorticoid receptors. Data on the reactivity of II and the stability of [3H]II-labeled receptors suggest that a cysteine-SH group has been labeled.
IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dexamethasone bromide)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

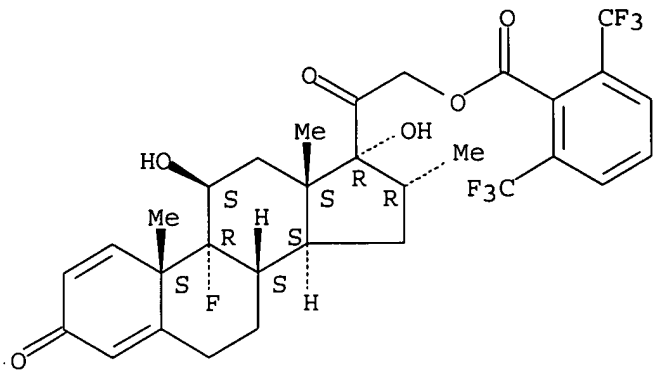


IT **131567-19-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and glucocorticoid receptor affinity of)
RN 131567-19-6 CAPLUS

10803578

CN Pregna-1,4-diene-3,20-dione, 21-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-9-fluoro-11,17-dihydroxy-16-methyl-, (11β,16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



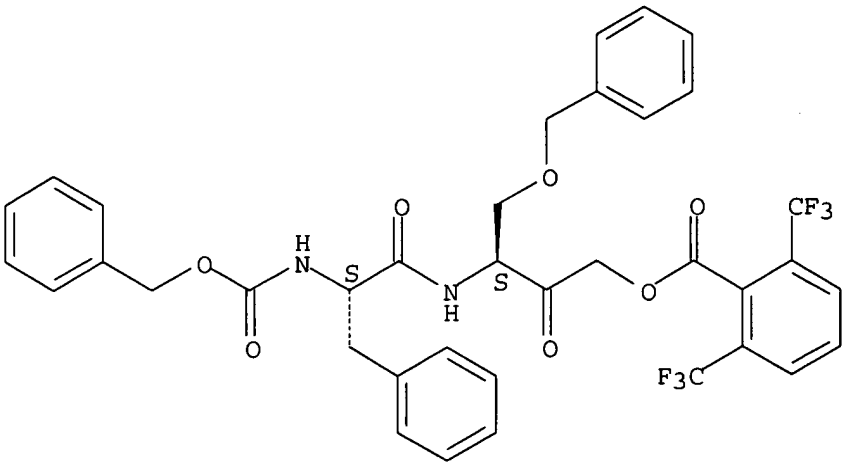
L3 ANSWER 109 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:224328 CAPLUS
DN 114:224328
TI Peptidyl (acyloxy)methyl ketones and the quiescent affinity label concept: the departing group as a variable structural element in the design of inactivators of cysteine proteinases
AU Krantz, Allen; Copp, Leslie J.; Coles, Peter J.; Smith, Roger A.; Heard, Stephen B.
CS Syntex Res. (Canada), Mississauga, ON, L5N 3X4, Can.
SO Biochemistry (1991), 30(19), 4678-87
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB (Acyloxy)methyl ketones, of general structure Z-[AA2]-[AA1]-CH2OCOAr (Z = benzyloxycarbonyl; AA = amino acid; Ar = aryl), were potent inactivators of the cysteine proteinase, cathepsin B. These reagents were designed as affinity labels in which the dipeptidyl moiety serves as an affinity group (complementary to the S1 and S2 sites of the enzyme), while the (acyloxy)methyl ketone unit (-COCH2OCOR), containing a weak leaving group in the form of a carboxylate nucleofuge, functions as the potentially reactive entity that labels the enzyme. The inhibition was time-dependent, active-site directed, and irreversible. The apparent 2nd-order rate constant (kinact/Kinact), which characterizes the inhibition of cathepsin B by this series, spanned several orders of magnitude and in certain cases exceeded 106 M-1 s-1. The activity of this series of inhibitors was found to be exquisitely sensitive to the nature of the carboxylate leaving group as well as the affinity group. A strong dependence of 2nd-order inactivation rate on leaving group pKa was uncovered for Z-Phe-Ala (acyloxy)methyl ketones [log(k/K) = -1.1 + pKa + 7.2. Heretofore, in constructing affinity labels the choice of leaving group was quite restricted. The aryl carboxylate group thus offers considerable variation as a design element in that both its binding affinity and reactivity can be controlled by substituent effects. Specific peptidyl (acyloxy)methyl ketones thus represent prime examples of highly potent, chemical stable enzyme inhibitors with variable structural elements in both the affinity and departing groups.
IT **115186-02-2 118253-03-5 118253-04-6**
133524-91-1 133577-39-6 133670-84-5
RL: BIOL (Biological study)

(cathepsin B inactivation by, structure in relation to)

RN 115186-02-2 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

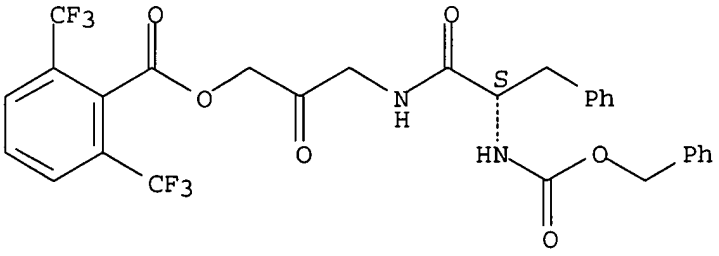
Absolute stereochemistry.



RN 118253-03-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]propyl ester (9CI) (CA INDEX NAME)

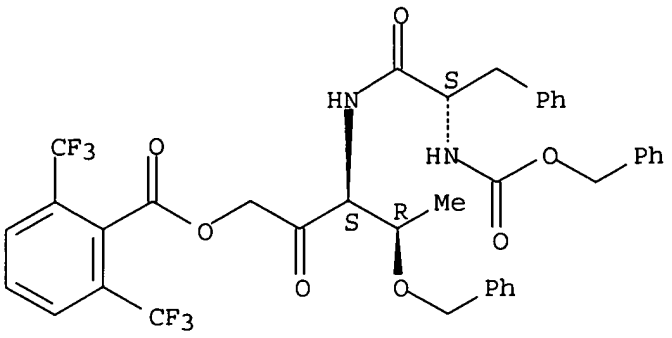
Absolute stereochemistry.



RN 118253-04-6 CAPLUS

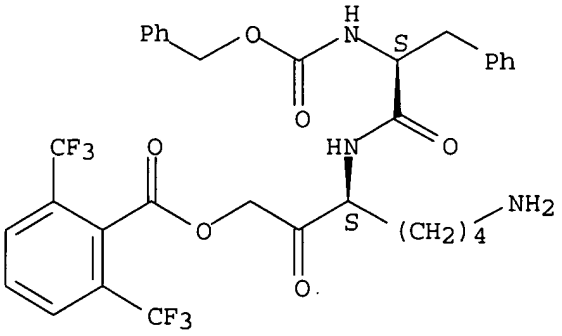
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)pentyl ester, [3S-[3R*(R*),4S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 133524-91-1 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 7-amino-2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]heptyl ester, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

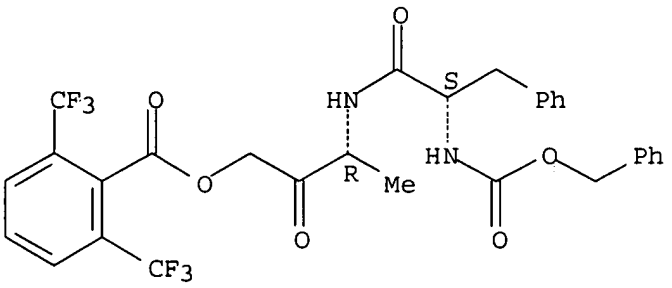
Absolute stereochemistry.



● HCl

RN 133577-39-6 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

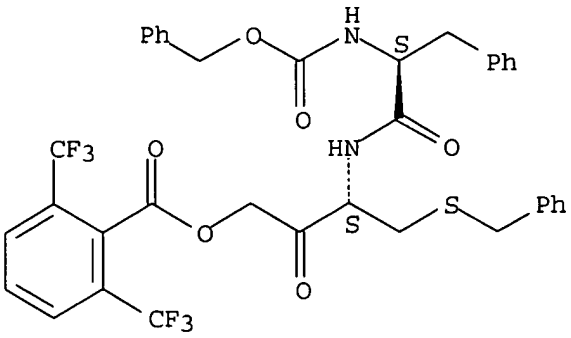


RN 133670-84-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-[(phenylmethyl)thio]butyl

10803578

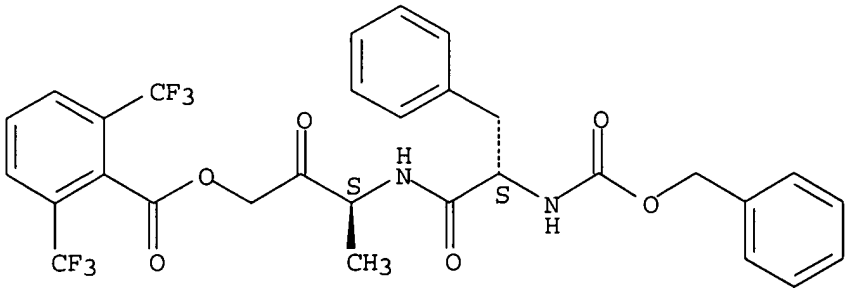
ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **115186-03-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cathepsin B inactivation by, structure in relation to)
RN 115186-03-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

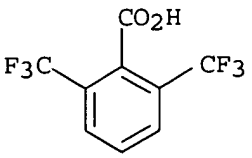
Absolute stereochemistry.



L3 ANSWER 110 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:206685 CAPLUS
DN 114:206685
TI Superbase reactions: the expedient and selective metalation of fluorine- or trifluoromethyl-substituted benzenes
AU Schlosser, Manfred; Katsoulos, Georges; Takagishi, Sadahito
CS Inst. Chim. Org., Univ. Lausanne, Lausanne, CH-1005, Switz.
SO Synlett (1990), (12), 747-8
CODEN: SYNLES; ISSN: 0936-5214
DT Journal
LA English
OS CASREACT 114:206685
AB When treated with the superbasic mixture of butyllithium and potassium tert-butoxide, fluorobenzene, difluorobenzenes, fluoro(trifluoromethyl)benzenes, (trifluoromethyl)benzene and bis(trifluoromethyl)benzenes undergo site-selective hydrogen-metal exchange. Best results are obtained in THF solns. at -75° or -50°. Upon quenching with carbon dioxide the corresponding carboxylic acids are obtained in good to excellent yield.
IT **24821-22-5P**, 2,6-Bis(trifluoromethyl)benzoic acid

10803578

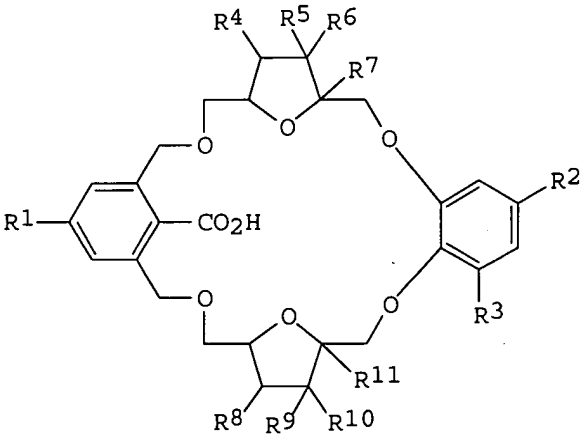
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 111 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:23990 CAPLUS
DN 114:23990
TI Preparation of tetrahydrofuran-containing macrocyclic polyether carboxylic acids as antibacterials and feed utilization enhancers
IN Urban, Frank J.
PA Pfizer Inc., USA
SO U.S., 24 pp. Cont. of U.S. Ser. No. 919,180, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4935442	A	19900619	US 1989-393832	19890814
PRAI US 1986-919180	B1	19860908		

OS MARPAT 114:23990
GI



I

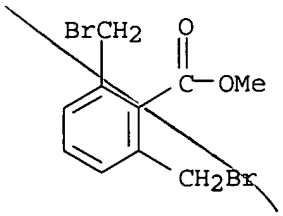
AB Title compds. I (R1 = H, Me3C; R2 = H, C1-10 alkyl, Ph; R3 = H, C1-8 alkyl, PhSCH2; R4-R11 = H, Me, provided that not more than 2 of R4-R7 = Me and not more than 2 of R8-R11 = Me) and their salts, useful as antibacterials and for increasing efficiency of feed utilization in ruminants, especially cattle (no data), were prepared The Me ester of I (R1 = Me3C; R2 = tert-C8H17; R3-R11 = H) was refluxed in aqueous EtOH containing KOH for

18 h to give I (R1 = Me3C, R2 = tert-C8H17; R3-R11 = H) as the K salt. The starting ester is prepared, e.g., by cyclization of a bis(bromomethyl)benzoate with the corresponding diol, itself derived from a catechol and a furan derivative Prepns. and properties of various precursors as well as I are described.

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of macrocyclic polyethers containing THF)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 112 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:552384 CAPLUS

DN 113:152384

TI The first internally functionalized chiral [2.2]metacyclophanes [Erratum to document cited in CA113(3):23876f]

AU Voegtle, Fritz; Ostrowicki, Andreas; Knops, Peter; Fischer, Peter; Rueter, Hans; Jansen, Martin

CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, Germany

SO Journal of the Chemical Society, Chemical Communications (1990), (6), 519
CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

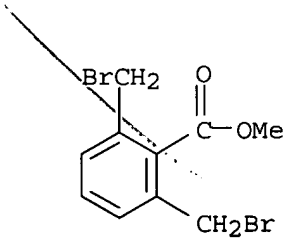
LA English

AB Errors in the text, Table 1, and Figure 3 have been corrected The errors were not reflected in the abstract or the index entries.

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with tosylaminobenzenethiol in presence of cesium ion (Erratum))

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 113 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:548383 CAPLUS

DN 113:148383

TI Use of fluorone derivatives in contrast media for cancerous growth diagnosis

IN Dzbanovskii, N. N.; Polsachev, V. I.; Potemkina, E. V.; Rakhimov, A. T.; Rubin, L. B.; Osipov, A. S.

PA Moscow State University, USSR

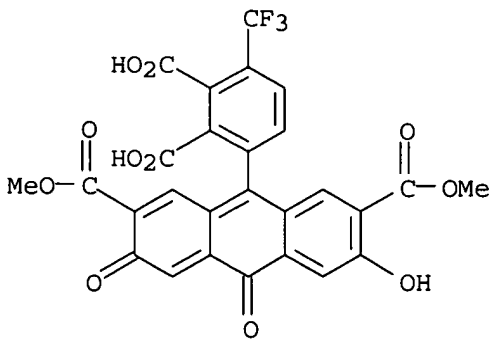
SO Eur. Pat. Appl., 31 pp.

10803578

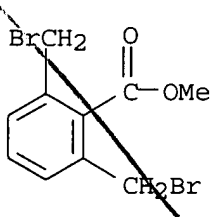
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 313942	A1	19890503	EP 1988-117157	19881014
	R: CH, DE, FR, GB, IT, LI, SE				
	FI 8804720	A	19890416	FI 1988-4720	19881013
	FI 8804721	A	19890416	FI 1988-4721	19881013
	NO 8804565	A	19890417	NO 1988-4565	19881013
	NO 8804566	A	19890417	NO 1988-4566	19881013
	JP 01211531	A2	19890824	JP 1988-257393	19881014
	JP 01221329	A2	19890904	JP 1988-257394	19881014
	EP 454185	A2	19911030	EP 1991-111514	19881014
	EP 454185	A3	19920108		
	R: CH, DE, FR, GB, IT, LI, SE				
	BR 8805356	A	19890613	BR 1988-5356	19881017
	BR 8805359	A	19890613	BR 1988-5359	19881017
	US 5093106	A	19920303	US 1990-485785	19900223
PRAI	SU 1987-4313068	A	19871015		
	US 1988-255120	B1	19881007		

OS MARPAT 113:148383
GI For diagram(s), see printed CA Issue.
AB Fluorone derivs. I [R1, R7 = H, halo, 131I, Me, CF3, CCl3, Et, CO2H, CO2Me, NO2, OH, OMe, OEt; R2, R4-R6 = H, halo, 131I, C1-5 (halo)hydrocarbyl, etc.; R3 = H, alkali metal cation, ammonium, etc.; R8 = H, C1-5 (substituted) alkyl, aminoacyl, etc.] are useful as contrast agents for x-ray, radio-, fluorescence, and NMR imaging of malignant neoplasms. They may be used alone or in combination with saccharides, disaccharides, vitamins, and/or cell-membrane permeability blockers (e.g. antihistaminics) to increase the accumulation of I in tumor cells. Thus, a contrast agent composition contained II (I; R1-R5 = R7 = H, R6 = CO2Et, R8 = 2-HO2CC6H4) 0.1, glucose 98.9, vitamin composition (retinol 1, thiamin 6, riboflavin 3, pyridoxine-HCl 6, rutin 6, tocopherol acetate 3, ascorbic acid 60, nicotinic acid 15%) 0.5, and 3-methyl-9-benzyl-1,2,3,4-tetrahydrocarboline naphthalene-1,5-disulfonate (membrane permeability blocker) 0.5 weight%. The accumulation of II from this composition by transplanted cervical carcinoma, Lewis tumor, and large intestinal carcinoma was 6.0-fold that by normal tissues.
IT **126491-22-3**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(as contrast agent, for neoplasm diagnosis)
RN 126491-22-3 CAPLUS
CN 2,7-Anthracenedicarboxylic acid, 9-[2,3-dicarboxy-4-(trifluoromethyl)phenyl]-3,10-dihydro-6-hydroxy-3,10-dioxo-, 2,7-dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 114 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:532147 CAPLUS
DN 113:132147
TI Intra- and extraannularly functionalized chiral [2.2]metacyclophanes synthesis, circular dichroism and structure/chiroptic relationships
AU Voegtle, Fritz; Knops, Peter; Ostrowicki, Andreas
CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Germany
SO Chemische Berichte (1990), 123(9), 1859-68
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 113:132147
GI For diagram(s), see printed CA Issue.
AB A simple one-step cyclization reaction of m-HSC6H4NHSO2C6H4Me-p with bis(bromomethyl)arenes for the synthesis of the title compds., e.g. I (R = Me, MeO, Ph) and II, is presented; separation (enrichment) of enantiomers is achieved by HPLC mainly on (+)-PTrMA. The kinetics of interconversion (racemization) of the new diheteral[2.2]metacyclophanes are determined: no racemization of the internally substituted phanes is found on heating until decomposition, whereas the extraannularly substituted compds. exhibit barriers of interconversion of about 130 kJ/mol, similar to that of the thiaazametacyclophane I (R = H). For the pyridinophane II the barrier (110 kJ/mol) is lower corresponding to the decreased spatial requirement of the nitrogen lone pair compared to a CH bond. The CD curves of the intraannularly functionalized phanes are compared with those of the extraannularly functionalized unsubstituted reference compds.: a bathochromic shift of the Cotton effect at short wavelengths is found, which is increasing with the bulkiness of the internal functional group.
IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with mercapto(tolylsulfonyl)aniline)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

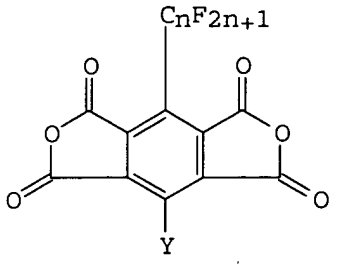


L3 ANSWER 115 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:460058 CAPLUS
DN 113:60058
TI Fluoroalkylpyromellitic anhydrides and their manufacture from durene derivatives
IN Ishizawa, Maki; Hasuda, Yoshiaki; Matsuura, Tooru
PA Nippon Telegraph and Telephone Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

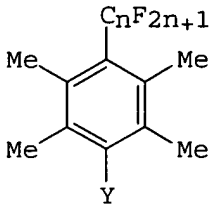
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02015084	A2	19900118	JP 1988-165056	19880704
	JP 2704200	B2	19980126		

10803578

PRAI JP 1988-165056 19880704
GI



I

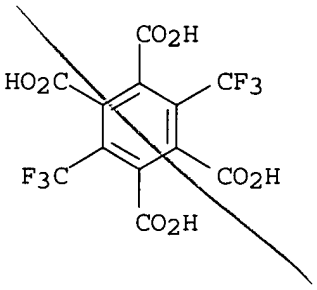


II

AB Title compds. I (Y = H, CnF2n+1;n = 1-10), useful for polyimide manufacture, are prepared by oxidation and dehydration of the corresponding durene derivs. II. Thus, heating 30 g diiododurene with 40 g CF3I over activated Cu in DMF at 150° gave 17.6 g di(trifluoromethyl)durene, which was oxidized in pyridine/H2O by dropwise addition of KMnO4 at 100°, then dehydrated in vacuo at 150° to give 10.3 g di(trifluoromethyl)pyromellitic anhydride (III). A mixture of 12.73 g III and 7.63 g o-tolidine was allowed to react in N-methylpyrrolidone at room temperature to give a polyamic acid, which was cast on an Al sheet and heated at
100°, 200°, and 350° to give a tough polyimide film.

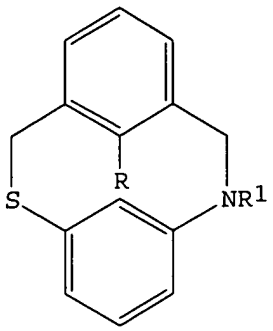
IT **128298-23-7P**
RL: PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(preparation and dehydration of)

RN 128298-23-7 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

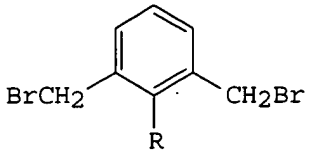


L3 ANSWER 116 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:423876 CAPLUS
DN 113:23876
TI The first internally functionalized chiral [2.2]metacyclophanes
AU Voegtle, Fritz; Ostrowicki, Andreas; Knops, Peter; Fischer, Peter; Reuter, Hans; Jansen, Martin
CS Inst. Org. Chem. Biochem., Universitat Bonn, Bonn, Fed. Rep. Ger.
SO Journal of the Chemical Society, Chemical Communications (1989), (22), 1757-9
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 113:23876
GI

10803578



I



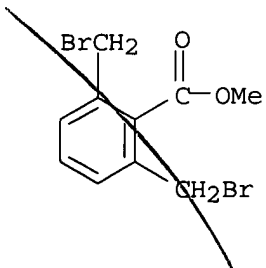
II

AB The new medium membered heterocycles I (R = Me, OMe, SMe, CO2Me, SO2Me, Ph, CMe3; R1 = tosyl), strained due to internal substituents, could be obtained after optimization of a simple one-step cyclization reaction of bis(bromomethyl)benzenes II with 3-HSC6H4NHR1 in presence of Cs+. The barrier of the restricted rotations of the Ph ring in I (R = Ph) and of the tert-Bu group in I (R = CMe3) were measured; the NMR and CD data of the stable enantiomers of I are compared with those of the less strained parent skeleton. The anti conformation of the aromatic rings of I (R = OMe, CO2Me, R1 = tosyl) were proven by x-ray crystal structure anal.

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with tosylaminobenzenethiol in presence of cesium ion)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 117 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:55828 CAPLUS

DN 112:55828

TI Lipophilic 1,3-xylyl-21-crown-6 macrocyclic polyether 2-carboxylic acids as biological mimics of the ionophore antibiotics

AU Urban, Frank J.; Chappel, Larry R.; Girard, Arthur E.; Mylari, Banavara L.; Pimblett, Ian J.

CS Pfizer Cent. Res., Groton, CT, 06340, USA

SO Journal of Medicinal Chemistry (1990), 33(2), 765-71
CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 112:55828

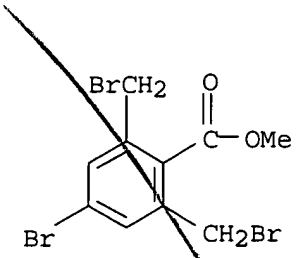
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

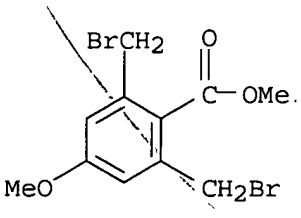
AB Twelve lipophilic 1,3-xylyl-21-crown-6 macrocyclic polyether 2-carboxylic acids, e.g. I (R = H, Me, PhCH2; n = 1), two lariat ether 1,3-xylyl-21-crown-6 macrocyclic polyether 2-carboxylic acids II (R1 = H, Me3C) and two 1,3-xyly-28-crown-8 macrocyclic polyether 2-carboxylic acids I (R = H, Me, n = 2) were synthesized and tested for in vitro antibacterial activity, in vitro stimulation of rumen propionic acid production, and in vivo anticoccidial activity in chickens. These are biol. screens relevant to animal health areas where the ionophore antibiotics such as monensin have found application. While the parent structure without lipophilic substituents was biol. inactive, the lipophilic macrocycles were active in the two in vitro tests but not against chicken coccidiosis. One compound I (R = Me, n = 1) was tested in cattle and was found to increase levels of propionic acid in the rumen fermentation This effect is considered an important factor for increasing the efficiency of feed utilization in cattle exhibited by the ionophore antibiotic monensin. The alkali ion salts of these lipophilic macrocyclic polyether carboxylic acids are very soluble in organic solvents and insol. in water. These compds. are proposed to act as ion-transport agents and functional mimics of the ionophore antibiotics in the biol. systems described above.

IT **124175-43-5P 124175-44-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with bis(hydroxyethoxyethoxy)benzenes)

RN 124175-43-5 CAPLUS
CN Benzoic acid, 4-bromo-2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



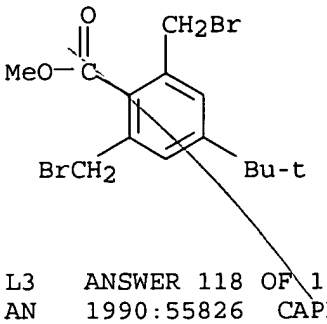
RN 124175-44-6 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)



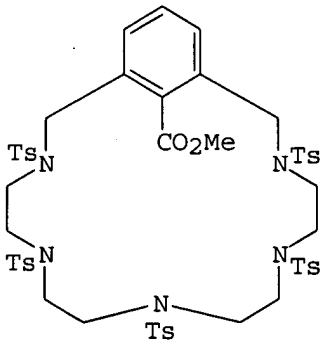
IT **119319-00-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 119319-00-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)

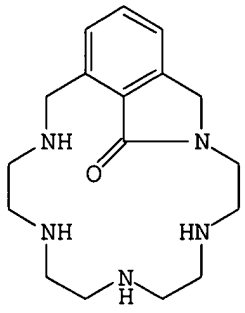
10803578



L3 ANSWER 118 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:55826 CAPLUS
DN 112:55826
TI Isolation and unusual stability of a new macrocyclic polyamine containing a phthalimidine
AU Kimura, Eiichi; Yoshiyama, Yukari; Shionoya, Mitsuhiko; Shiro, Motoo
CS Inst. Mol. Sci., Okazaki Natl. Res. Inst., Okazaki, 444, Japan
SO Journal of Organic Chemistry (1990), 55(2), 764-6
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 112:55826
GI



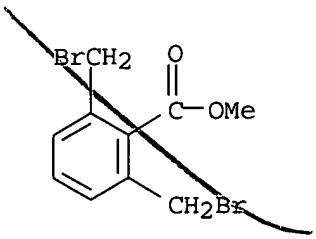
I



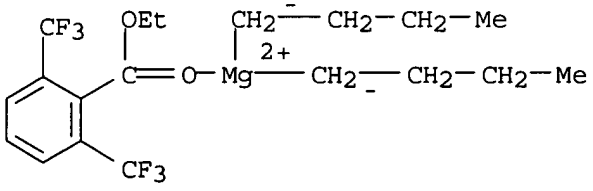
II

AB Cyclocondensation of 2,6-(BrCH2)2C6H3CO2Me with (TsNHCH2CH2NTsCH2CH2)2NTs (Ts = 4-MeC6H4SO2) in the presence of NaH in DMF gave 70% the pentatosyl macrocyclic carboxylate I. Treating the latter compound with 45% HBr in AcOH followed by ion exchange gave 28% the title compound II. The expected detosylated carboxylate could not be isolated due to the unusual reactivity of its carbonyl and the exceptional stability of II. The structure of II was confirmed by x-ray crystal anal.
IT **56263-51-5**, Methyl 2,6-bis(bromomethyl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with pentatosyl pentaamine derivative)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 119 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:21326 CAPLUS
DN 112:21326
TI Supported propene polymerization catalysts. 1. Supports derived from magnesium dialkyl-sterically hindered aromatic ester complexes
AU Johnson, Bryce V.; Karayannis, Nicholas M.; Hoppin, Charles R.; Ornellas, Linda; Khelghatian, Habet M.
CS Amoco Chem. Co., Naperville, IL, 60566, USA
SO Makromolekulare Chemie (1989), 190(8), 1997-2007
CODEN: MACEAK; ISSN: 0025-116X
DT Journal
LA English
AB Highly active supported propene polymerization catalysts are prepared by activating
supports derived from Mg dialkyl complexes with sterically hindered aromatic esters, such as Et 2,6-dimethylbenzoate, Et 2,4,6-trimethylbenzoate (I), or iso-PrOBz. The support is precipitated by reacting a hexane solution of the Mg
dialkyl complex with SiCl4 and then activated by treatment with TiCl4 and diisobutyl phthalate in PhCl. Optimized catalysts of this type prepared from Mg dialkyl complex with I realize yields of 16-17 kg isotactic polypropylene/g catalyst in 2 h hexane slurry polymns. at 70°/10.2 atm, with <1% boiling hexane extractables and 0.41-0.43 g/mL polymer powder bulk d. The cocatalyst-external modifier package used consists of AlEt3-(MeO)2SiPh2. The polymer produced is characterized by a narrow particle size distribution.
IT **124273-08-1**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polymerization of propylene)
RN 124273-08-1 CAPLUS
CN Magnesium, dibutyl[ethyl 2,6-bis(trifluoromethyl)benzoate-O']- (9CI) (CA INDEX NAME)



L3 ANSWER 120 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:615900 CAPLUS
DN 111:215900
TI Polyimide precursors
IN Kunugi, Katsuo; Saiki, Noritsugu
PA Teijin Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF

10803578

DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01108227	A2	19890425	JP 1987-267308	19871021
PRAI	JP 1987-267308		19871021		

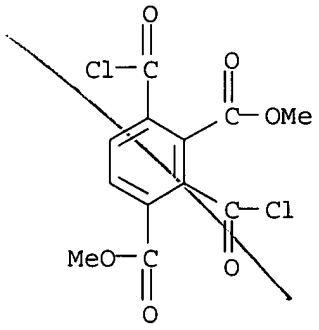
AB Precursors for polyimide fibers and films contain ≥80 mol% aromatic tetracarboxylic acid diester-aromatic diamine condensates and aromatic tetracarboxylic acid-aromatic diamine condensates. Stirring 2.51 g p-phenylenediamine in 150 mL N-methylpyrrolidone (I) with 2.53 g pyromellitic dianhydride at -10° and then with 3.70 g 1:1 mixture of 2,5-dicarbomethoxyterephthaloyl chloride and 2,4-dicarbomethoxyisophthaloyl chloride gave a polyamic acid which was dry spun into aqueous I, drawn 2-fold in air, cyclized in Ac2O-pyridine for 24 h, dried, and drawn 1.23-fold at 250° and 520° to give fibers with tenacity 12.1 g/denier, elongation 1.3%, and initial modulus 1200 g/denier.

IT **123745-99-3P**
RL: PREP (Preparation)
(manufacture of, for fibers and films)

RN 123745-99-3 CAPLUS
CN 1,3-Benzenedicarboxylic acid, 2,4-bis(chlorocarbonyl)-, dimethyl ester, polymer with 1,4-benzenediamine, 1H,3H-benzo[1,2-c:4,5-c']difuran-1,3,5,7-tetrone and dimethyl 2,5-bis(chlorocarbonyl)-1,4-benzenedicarboxylate (9CI) (CA INDEX NAME)

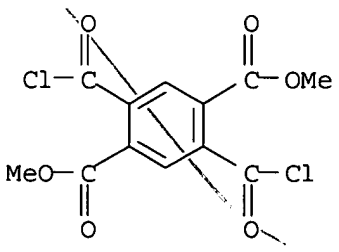
CM 1

CRN 19116-49-5
CMF C12 H8 Cl2 O6



CM 2

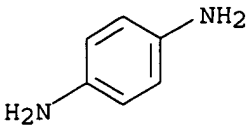
CRN 19014-14-3
CMF C12 H8 Cl2 O6



10803578

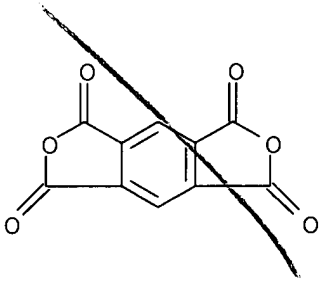
CM 3

CRN 106-50-3
CMF C6 H8 N2



CM 4

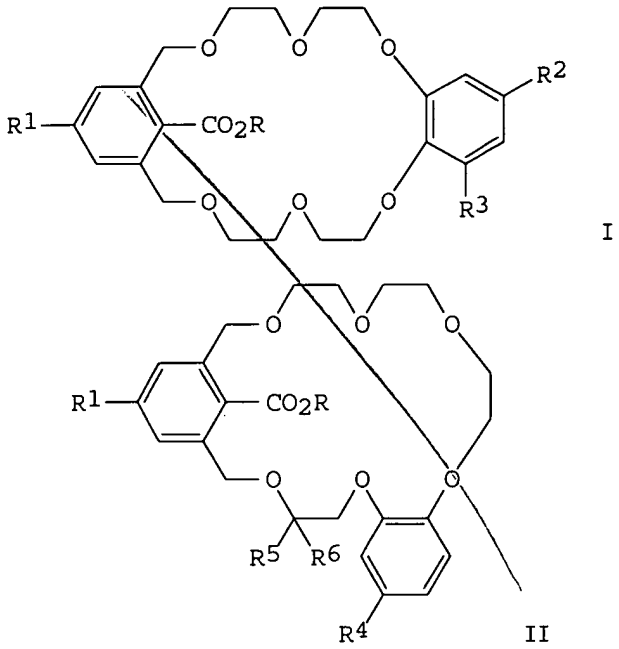
CRN 89-32-7
CMF C10 H2 O6



L3 ANSWER 121 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:457764 CAPLUS
DN 111:57764
TI Preparation of macrocyclic polyether carboxylic acids as enhancers of feed utilization efficiency
IN Urban, Frank J.
PA Pfizer Inc., USA
SO U.S., 25 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4777270	A	19881011	US 1986-916676	19860904
	WO 9313089	A1	19930708	WO 1985-US109	19850122
	W: US				
	US 4876367	A	19891024	US 1988-241169	19880906
PRAI	WO 1985-US109	W	19850122		
	US 1986-916676	A3	19860904		

OS CASREACT 111:57764; MARPAT 111:57764
GI



I

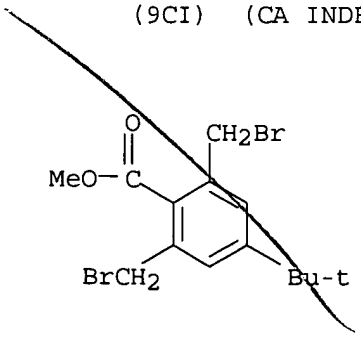
II

AB The title compds. [I, II; R = H; R1 = H, Me3C; R2 = H, C1-14 alkyl, C5-8 cycloalkyl, 1-adamantyl, C1-4 alkylphenyl, (un)substituted Me3CCH2CH2CHPh, Me3CCH:CPh; R3 = H, C1-8 alkyl, HOCH2, MeOCH2, (un)substituted phenylalkyl, PhCH2OCH2, PhSCH2, (pyridinylthio)methyl; R4 = H, C1-8 alkyl; R5 = H; R6 = H, C1-8 alkyl, PhSCH2 (un)substituted PhOCH2; R5R6 = cyclohexylidene], and their salts, especially I (R = H; R1 = H, Me3C; R2 = Me3CCH2CMe2; R4 = R7R8C6H3SCH2; R7, R8 = H, C1-3 alkyl, C1-3 alkoxy, C1-3 alkylthio, Br, Cl, F, CF3, OH, MeCO, PhCO, AcNH), were prepared as enhancers of ruminant feed utilization efficiency (no data). Thus, 3-(morpholinomethyl)-5-tert-octylpyrocatechol was etherified with 2-(2-chloroethoxy)ethyl tetrahydropyranyl ether and the product was deprotected and cyclocondensed with Me 2,6-bis(bromomethyl)-4-tert-butylbenzoate to give I (R = Me, R1 = Me3C, R2 = Me3CCH2CMe2, R3 = morpholinomethyl). The latter was converted in 4 steps to I [R3 = (2-pyridylthio)methyl, other groups unchanged] which was saponified in aqueous KOH, followed by acidification, to give I [R = H, R1 = Me3C, R2 = Me3CCH2CMe2, R3 = (2-pyrimidylthio)methyl]. more than 100 I (R = H, K) were prepared

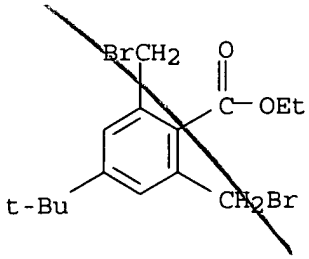
IT **119319-00-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of feed additives)

RN 119319-00-5 CAPLUS

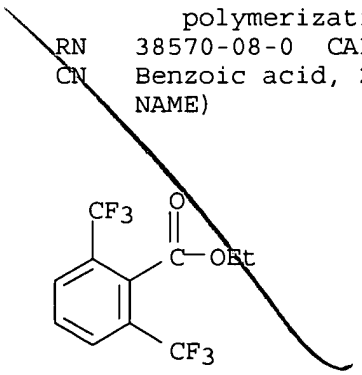
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, methyl ester (9CI) (CA INDEX NAME)



IT **119318-52-4**, Ethyl 2,6-bis(bromomethyl)-4-tert-butylbenzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of feed additives)
RN 119318-52-4 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-4-(1,1-dimethylethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 122 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:213419 CAPLUS
DN 110:213419
TI Highly active supported propylene polymerization catalysts prepared by activation of supports derived from precomplexed magnesium alkyls
AU Karayannis, N. M.; Johnson, B. V.; Hoppin, C. R.; Khelghatian, H. M.
CS Amoco Chem. Co., Naperville, IL, 60566, USA
SO Transition Met. Organomet. Catal. Olefin Polym., [Proc. Int. Symp.] (1988), Meeting Date 1987, 231-7. Editor(s): Kaminsky, Walter; Sinn, Hansjoerg. Publisher: Springer, Berlin, Fed. Rep. Ger.
CODEN: 56LAAQ
DT Conference
LA English
AB TiCl4-AlEt3-diisobutyl phthalate catalysts had good activity in propene polymerization when their dibutyl- or butyloctylmagnesium supports were first complexed with Et 2,6-dimethylbenzoate, Et 2,4,6-trimethylbenzoate, iso-Pr benzoate, or di-Bu butylphosphonate, before addition of the catalysts. The supported catalysts thus prepared had activities ≤17 kg/g catalyst in slurry polymns. of propene at 70° and 10.2 atm monomer for 2 h.
IT **38570-08-0D**, Ethyl 2,6-bis(trifluoromethyl)benzoate, reaction products with dialkylmagnesium
RL: USES (Uses)
(supports, containing silicon tetrachloride, for titanium tetrachloride-triethylaluminum-diisobutyl phthalate catalysts, in polymerization of propene)
RN 38570-08-0 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 123 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:135219 CAPLUS
DN 110:135219
TI Synthesis of 2,4(5)-bis(hydroxymethyl)imidazoles and 2,4(5)-bis[(2-hydroxyethoxy)methyl]imidazoles. Precursors of 2,4(5)-connected imidazole

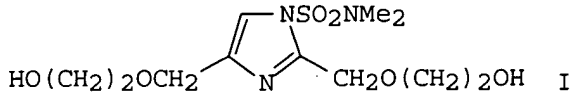
10803578

crown ethers

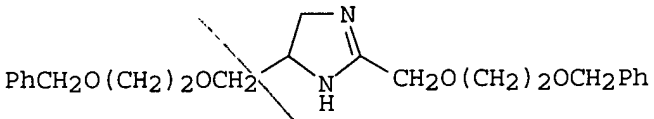
AU Zimmerman, Steven C.; Cramer, Katherine D.; Galan, Adam A.
CS Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA

SO Journal of Organic Chemistry (1989), 54(6), 1256-64
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 110:135219

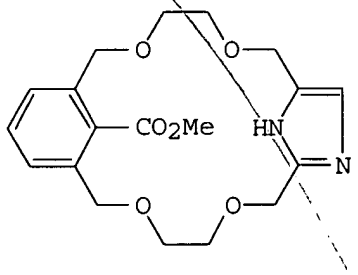
GI



I



II



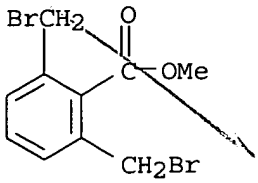
III

AB Two syntheses of 1-[(dimethylamino)sulfonyl]-2,4-bis[(2-hydroxyethoxy)methyl]imidazole, I, a precursor to imidazole-containing crown ethers, are described. The first involved hydroxymethylation of 1-benzylimidazole with formaldehyde to afford 1-benzyl-2,5-bis(hydroxymethyl)imidazole (20% yield), which was elaborated into I in four steps. An alternative and more efficient route involved coupling of PhCH2O(CH2)2OCH2CH(NH2)CH2NH2 with the imino ether obtained from PhCH2O(CH2)2OCH2CN to afford imidazoline II. The imidazoline was oxidized under Swern conditions, providing a mild new method of imidazole synthesis. Sulfamylation and debenzylation produced I. This approach was also applied to the synthesis of 1-[(dimethylamino)sulfonyl]-2,4-bis(hydroxymethyl)imidazole. Diol I was converted into 2,4-connected imidazole crown ethers, e.g., III, which formed a crystalline complex with water. The complex structure was determined by x-ray crystallog.

IT **56263-51-5**, Methyl 2,6-bis(bromomethyl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with bis(hydroxyethoxymethyl)imidazole, crown ether from)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

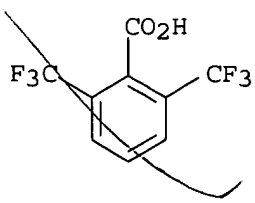
10803578



L3 ANSWER 124 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:39372 CAPLUS
DN 110:39372
TI Preparation and testing of peptidyl aryloxymethyl (or arylacyloxymethyl) ketones as thiol protease inhibitors
IN Krantz, Alexander; Pauls, Heinz W.; Smith, Roger A.; Spencer, Robin W.
PA Syntex Corp., Can.
SO Eur. Pat. Appl., 43 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 272671	A2	19880629	EP 1987-118949	19871221
	EP 272671	A3	19900613		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 5055451	A	19911008	US 1987-127282	19871207
	DK 8706743	A	19880623	DK 1987-6743	19871221
	AU 8782871	A1	19880721	AU 1987-82871	19871221
	AU 602547	B2	19901018		
	JP 63253061	A2	19881020	JP 1987-325156	19871221
	ZA 8709577	A	19890830	ZA 1987-9577	19871221
	AT 102951	E	19940415	AT 1987-118949	19871221
	CA 1329862	A1	19940524	CA 1987-554950	19871221
	ES 2061480	T3	19941216	ES 1987-118949	19871221
	US 5158936	A	19921027	US 1991-700686	19910515
PRAI	US 1986-946737	A	19861222		
	US 1987-127282	A	19871207		
	EP 1987-118949	A	19871221		

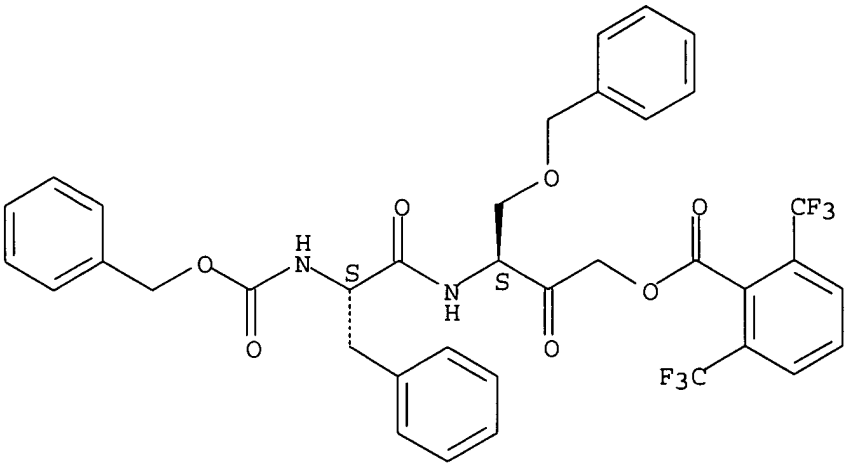
OS MARPAT 110:39372
AB XYnNHCHRCOCH2O(CO)n R1 [I; R = (protected) α-amino acid side chain; R1 = (substituted) aryl; X = H, N-protecting group; Y = (protected) α-amino acid residue; n = 0, 1; n = 0-2] useful as serine protease inhibitors, were prepared PhCH2O2C-Phe-Thr(CH2Ph)CH2Br (preparation given) and pentafluorophenol in DMF were stirred with K2CO3 and Bu4NI to give 85% PhCH2O2(-Phe-Thr(CH2Ph)CH2OC6F5. I at 100 mg/kg i.v. in rats gave 97-100% inhibition of cathepsin B.
IT **24821-22-5**, 2,6-Bis(trifluoromethyl)benzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylalanylalanine bromomethyl ketone, in preparation of thiol protease inhibitor)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



IT **115186-02-2P 115186-03-3P 118237-64-2P**
118252-86-1P 118252-88-3P 118252-89-4P
118253-03-5P 118253-04-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as thiol protease inhibitor)

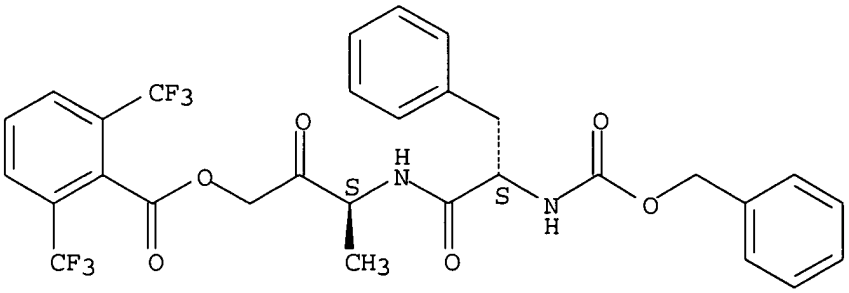
RN 115186-02-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



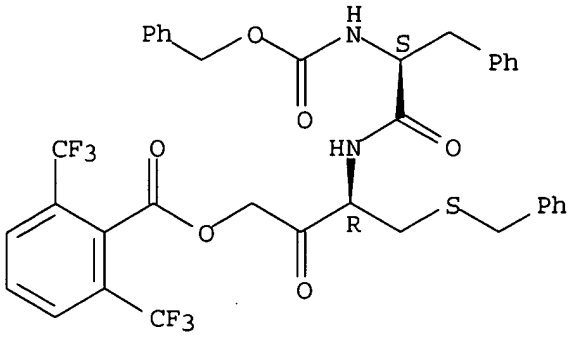
RN 115186-03-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



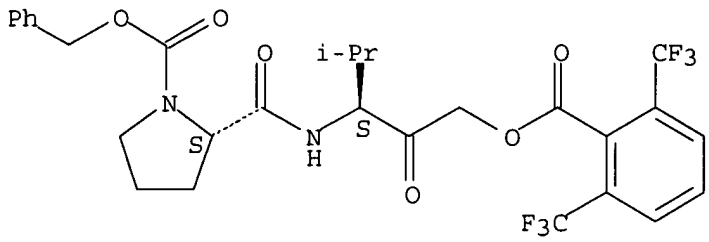
RN 118237-64-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-[(phenylmethyl)thio]butyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



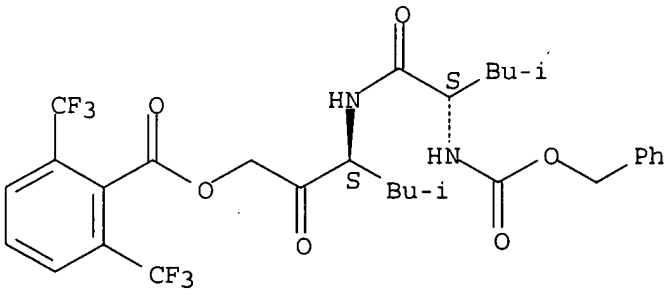
RN 118252-86-1 CAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(1-methylethyl)-2-oxopropyl]amino]carbonyl]-, phenylmethyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



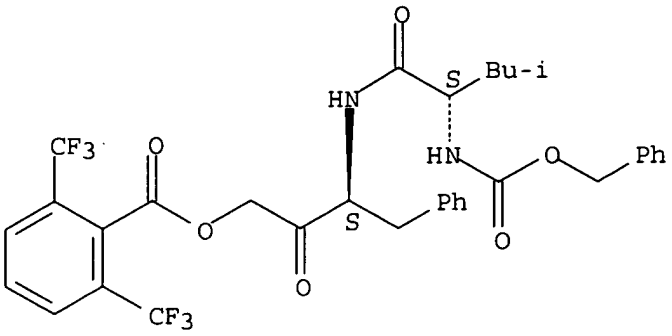
RN 118252-88-3 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 5-methyl-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-2-oxohexyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



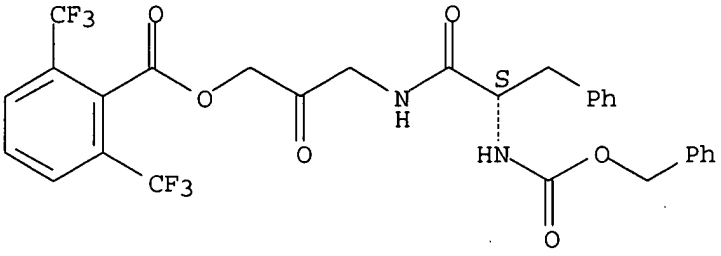
RN 118252-89-4 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-2-oxo-4-phenylbutyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



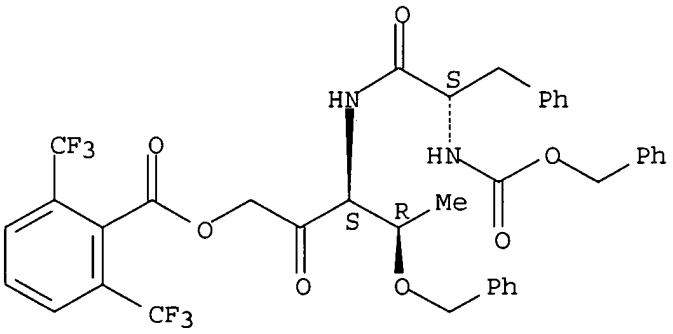
RN 118253-03-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 118253-04-6 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)pentyl ester, [3S-[3R*(R*),4S*]]- (9CI) (CA INDEX NAME)

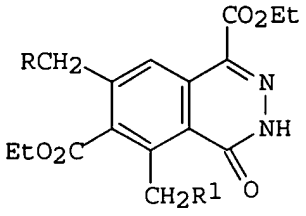
Absolute stereochemistry.



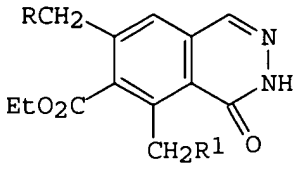
L3 ANSWER 125 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1989:8145 CAPLUS
DN 110:8145
TI Synthesis of antiatherosclerotic agents. XIII. Synthesis of phthalazinol derivatives
AU Eguchi, Yukuo; Hasegawa, Yuko; Katano, Emiko; Komoda, Yasuo; Ishikawa, Masayuki

10803578

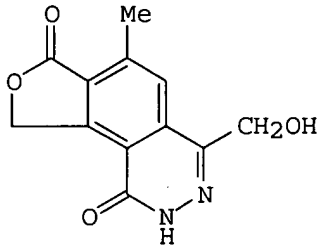
CS Inst. Med. Dent. Eng., Tokyo Med. Dent. Univ., Tokyo, 101, Japan
SO Iyo Kizai Kenkyusho Hokoku (Tokyo Ika Shika Daigaku) (1987), 21, 27-33
CODEN: IKKHBS; ISSN: 0082-4739
DT Journal
LA Japanese
GI



I



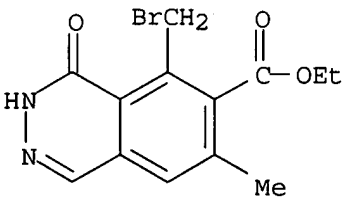
II



III

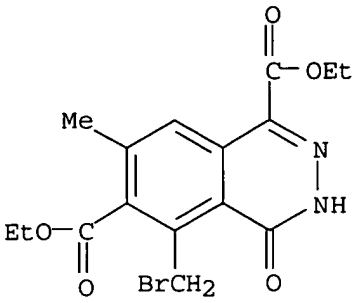
AB Bromination of dicarbethoxydimethylphthalazinone I (R = R1 = H) gave 48% I (R = H, R1 = Br) and 4% I (R = R1 = Br). I (R = H, R1 = Br) was converted to 5 carbethoxyphthalazinone derivs. II (R = H, R1 = Br, OMe, piperidino, cyano) and III. I (R = R1 = Br) was treated with AgNO3-MeOH and then NaBH4 to give II (R = R1 = OMe). These II and III were tested for inhibition of platelet aggregation, but none showed activity as high as that of II (R = R1 = H).

IT **118006-08-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and blood platelet aggregation inhibition of)
RN 118006-08-9 CAPLUS
CN 6-Phthalazinecarboxylic acid, 5-(bromomethyl)-3,4-dihydro-7-methyl-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

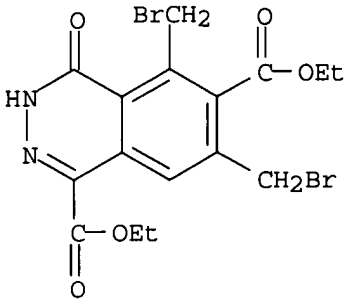


IT **56611-74-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
RN 56611-74-6 CAPLUS
CN 1,6-Phthalazinedicarboxylic acid, 5-(bromomethyl)-3,4-dihydro-7-methyl-4-oxo-, diethyl ester (9CI) (CA INDEX NAME)

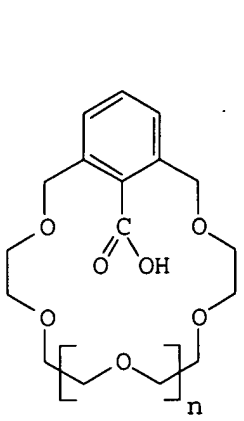
10803578



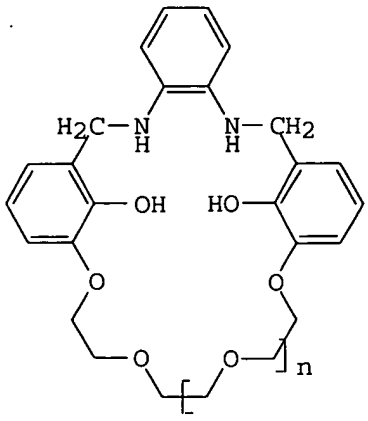
IT **118006-07-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, decarbethoxylation and methoxylation of)
RN 118006-07-8 CAPLUS
CN 1,6-Phthalazinedicarboxylic acid, 5,7-bis(bromomethyl)-3,4-dihydro-4-oxo-, diethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 126 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:630151 CAPLUS
DN 109:230151
TI Synthetic molecular receptors for urea. Macrocyclic ligands with intraannular acidic groups and the complexes with urea
AU Van Staveren, Catherina J.; Aarts, Veronika M. L. J.; Grootenhuis, Peter D. J.; Droppers, Wichert J. H.; Van Eerden, Johan; Harkema, Sybolt; Reinhoudt, David N.
CS Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.
SO Journal of the American Chemical Society (1988), 110(24), 8134-44
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 109:230151
GI



I



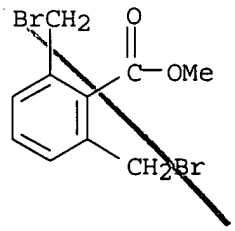
II

AB Measurements of the acidities of macrocycles containing intraannular acidic groups provide a method to evaluate the complexation of these crown ethers with neutral mols. in polar media. Six types of crown ethers with intraannular pyridinium, phenolic, and/or carboxylic groups were synthesized. Complexation with urea was assessed by accurate potentiometric titrns., liquid-liquid or solid-liquid extraction, and x-ray crystallog. In solid-liquid extns., efficiencies of complexation of urea by the macrocycles of ≤0.54 were found. In liquid-liquid extns., competition with water caused lower extraction efficiencies. The crystal structures of 2-carboxy-1,3-xylyl-24-crown-7.H2O [I (n = 3).H2O], 2-carboxy-1,3-xylyl-30-crown-9.urea [I (n = 5).urea], and II (n = 4).urea are reported. All these structures show encapsulation of the guest and prove that the acidic groups are involved in H bonding to the guest.

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(macrocyclization of, with (polyoxaalkanediyl)bis(pyridinemethanol) derivs.)

RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 127 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:612513 CAPLUS
DN 109:212513
TI Fluorine-containing polyamic acids and polyimides for coatings
IN Numata, Shunichi; Fujisaki, Koji; Kinjo, Noriyuki
PA Hitachi, Ltd., Japan; Hitachi Chemical Co., Ltd.
SO U.S., 15 pp. Division of U.S. Ser. No. 670,977, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4760126	A	19880726	US 1986-904203	19860908

10803578

PRAI US 1984-670977 A3 19841113

AB The title polymers, heat- and moisture-resistant, are prepared from dianhydrides containing perfluoroalkylidene groups and diamines. Stirring 12.95 g bisphenol AF trimellitic anhydride ester (1:2), 2.05 g p-phenylenediamine (I), and 85 g N-methylpyrrolidone at room temperature for 5 h
(viscosity 250 P at 25°) gave a polyamic acid solution which was coated on glass and heated at 150° for 1 h, 250° for 30 min, and 400° for 1 h to give a polyimide with good heat resistance and moisture absorption (25°, relative humidity 75%) 0.75%; vs. good and 4.8, resp., for pyromellitic dianhydride -I polyimide.

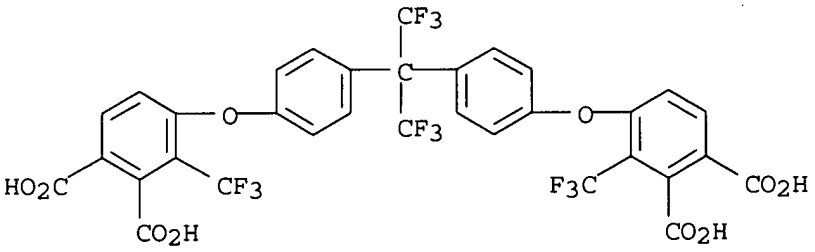
IT **98180-60-0P 117579-21-2P**
RL: TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(coatings, heat- and moisture-resistant, manufacture of)

RN 98180-60-0 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[3-(trifluoromethyl)-, polymer with 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[benzenamine] (9CI) (CA INDEX NAME)

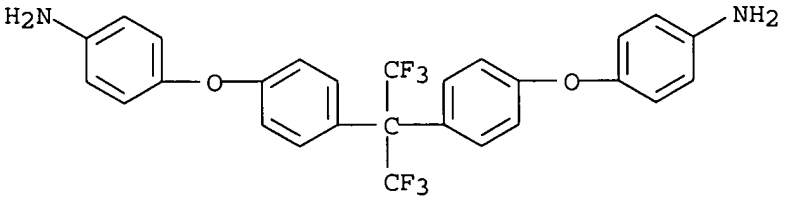
CM 1

CRN 98180-59-7
CMF C33 H16 F12 O10



CM 2

CRN 69563-88-8
CMF C27 H20 F6 N2 O2

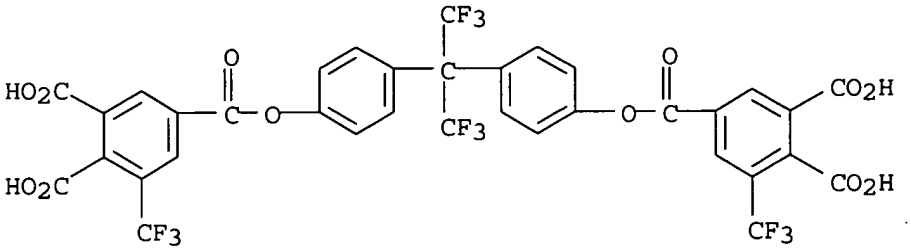


RN 117579-21-2 CAPLUS

CN 1,2,4-Benzenetricarboxylic acid, 6-(trifluoromethyl)-, 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]di-4,1-phenylene] ester, polymer with 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[benzenamine] (9CI) (CA INDEX NAME)

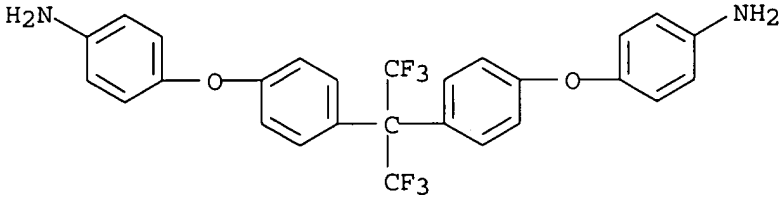
CM 1

CRN 117579-20-1
CMF C35 H16 F12 O12

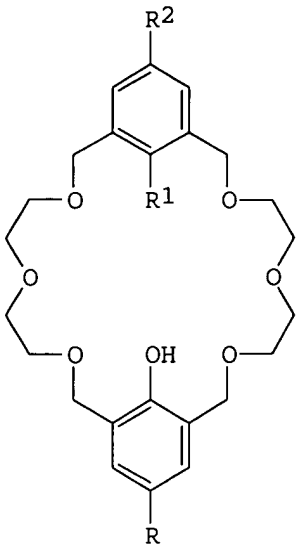


CM 2

CRN 69563-88-8
CMF C27 H20 F6 N2 O2



L3 ANSWER 128 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:473412 CAPLUS
DN 109:73412
TI Synthesis, coloration, and crystal structure of the dibasic chromoacerand-piperazine 1:1 salt complex
AU Kaneda, Takahiro; Ishizaki, Yuka; Misumi, Soichi; Kai, Yasushi; Hirao, Gen; Kasai, Nobutami
CS Inst. Sci. Ind. Res., Osaka Univ., Ibaraki, 567, Japan
SO Journal of the American Chemical Society (1988), 110(9), 2970-2
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CASREACT 109:73412
GI

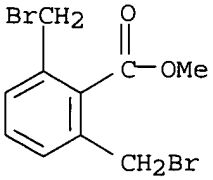


I

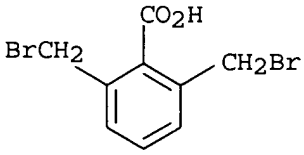
AB Three new chromoacerands I [R = N:NC6H3(NO2)2-2,4; R1 = CO2H (II), CO2Me, R2 = H; R1 = R2 = OMe] were prepared to examine their amine-selective coloration. The salts of II with diamines such as piperazines exhibited tremendously blue-shifted absorption maximum compared with bulky monoamines such as Pr3N. The crystal structure of the II-piperazine 1:1 salt complex revealed a good fit of the piperazinium cation in the cavity and the existence of a strong N+H-O- H-bond between an axial NH of the guest and the phenolate O of the host. The observed blue-shift in the II-piperazine system was correlated to this H-bonding and the association constant was determined spectrophotometrically.

IT **56263-51-5 56263-54-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with crown ether precursor)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 56263-54-8 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)- (9CI) (CA INDEX NAME)

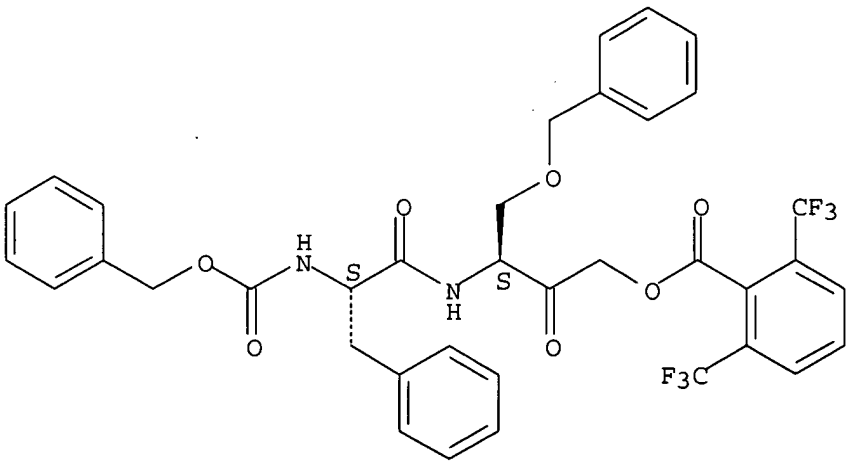


L3 ANSWER 129 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

10803578

AN 1988:434384 CAPLUS
DN 109:34384
TI New inhibitors of cysteine proteinases. Peptidyl acyloxymethyl ketones and the quiescent nucleofuge strategy
AU Smith, Roger A.; Copp, Leslie J.; Coles, Peter J.; Pauls, Henry W.; Robinson, Valerie J.; Spencer, Robin W.; Heard, Stephen B.; Krantz, Allen
CS Syntex Res. (Canada), Mississauga, ON, L5N 3X4, Can.
SO Journal of the American Chemical Society (1988), 110(13), 4429-31
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB Peptidyl acyloxymethyl ketones are potent and specific inhibitors of the cysteine proteinase, cathepsin B. These inhibitors are affinity labels in which the peptide moiety serves to transport an aryl carboxylate nucleofuge that is uniquely reactive toward the active-site cysteine thiol of the target enzyme. Heretofore, in constructing affinity labels the choice of leaving group was severely restricted. The aryl carboxylate group offers considerable variation as a design element in that its binding affinity and reactivity can be controlled by substituent effects. The apparent 2nd-order rate constant which characterizes the inhibition of bovine spleen cathepsin B by this series spans several orders of magnitude and in certain cases exceeds 106 M-1 s-1. The inhibition is time-dependent, active-site directed, and irreversible. The inactivation requires that the peptide component contain high affinity recognition elements for this enzyme and that the aryl carboxylate leaving group has a pKa <4. Impressive inhibitory activity is also observed for certain peptidyl aryloxymethyl ketones. NMR resonances of the inactivated adduct resulting from the action of representative 13C-labeled acyloxymethyl and aryloxymethyl ketone inhibitors on the model cysteine proteinase papain are consistent with the proposed mechanism of inactivation, involving displacement of the nucleofuge by the active-site cysteine to give a (cysteine-25)-thiomethyl ketone.
IT **115186-02-2P 115186-03-3P 115186-19-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of cathepsin B inhibition by)
RN 115186-02-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-4-(phenylmethoxy)butyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

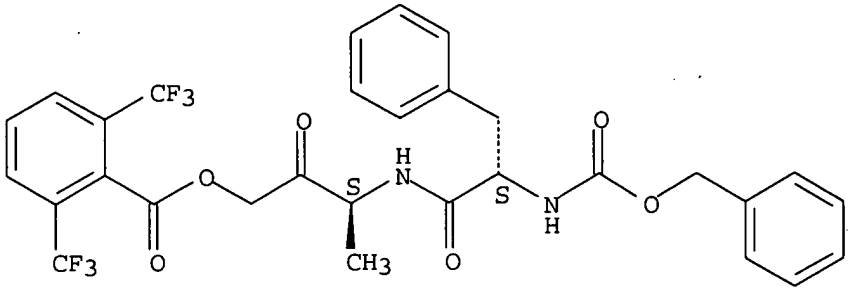


RN 115186-03-3 CAPLUS

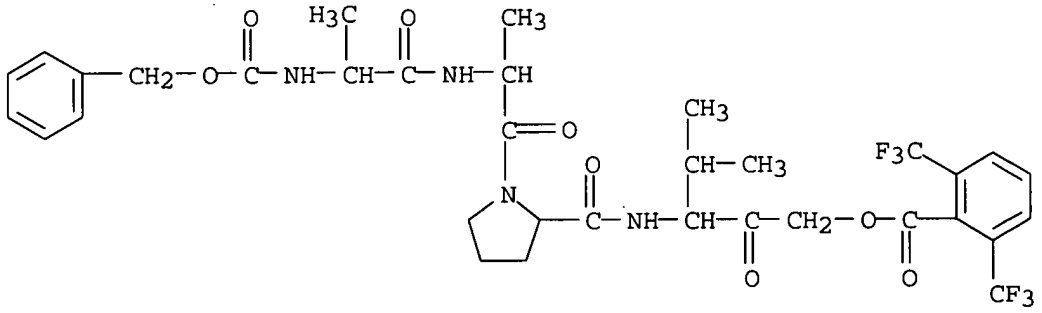
10803578

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]butyl ester, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

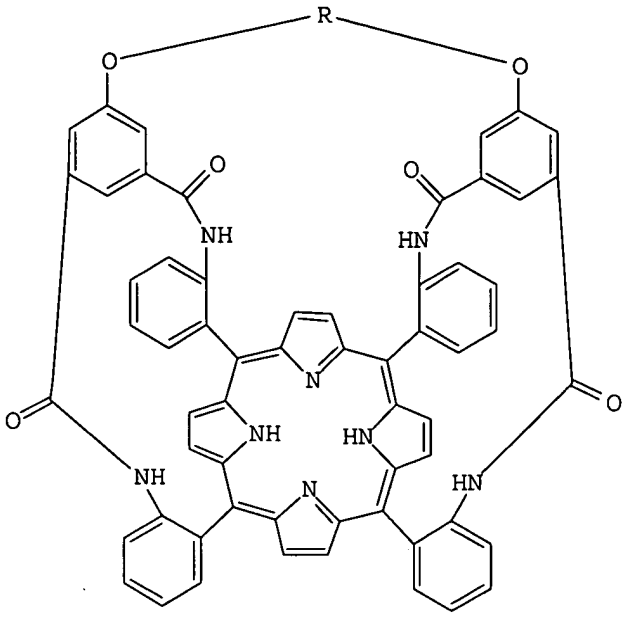
Absolute stereochemistry.



RN 115186-19-1 CAPLUS
CN L-Prolinamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-alanyl-N-[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(1-methylethyl)-2-oxopropyl]-, (S)-(9CI) (CA INDEX NAME)



L3 ANSWER 130 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:215215 CAPLUS
DN 108:215215
TI Synthesis, characterization, and x-ray structure of the ruthenium picnic-basket porphyrins
AU Collman, James P.; Brauman, John I.; Fitzgerald, Jeffrey P.; Hampton, Philip D.; Naruta, Yoshinori; Sparapany, John W.; Ibers, James A.
CS Dep. Chem., Stanford Univ., Stanford, CA, 94305, USA
SO Journal of the American Chemical Society (1988), 110(11), 3477-86
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
GI



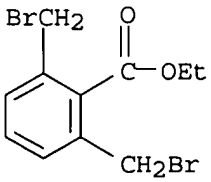
I

AB The convergent and general preparation and characterization are presented of a new class of sterically protected porphyrins, the picnic-basket porphyrins I [R = (CH2)n (n = 2, 4, 6, 8, 10), p-xylene, EtO2CC6H3(CH2)2-2,6, and 1,1'-binaphthyl-2,2'-diylbis(oxyethyl)]. I, which were prepared as cytochrome P 450 active-site analogs, bear a rigid superstructure on 1 face of the porphyrin macrocycle. The cavity defined by the appended superstructure may be readily varied in size, chirality, and functionality. The preparation and characterization, including an X-ray structure, of several Ru picnic-basket porphyrin carbonyl complexes are reported. The regiochem. of axial ligation in these Ru derivs. was determined by 1H NMR spectroscopy. RuQ(CO)(py) (Q = I; R = (CH2)6), in which CO is in the cavity and pyridine is outside the cavity, is monoclinic, space group P21/n, with a 16.112(7), b 18.687(7), c 24.750(7) Å, β 92.83(2)°, Z = 4, d.(calculated) = 1.402 g cm-3, R = 0.069, Rw = 0.066.

IT **113585-50-5P**, Ethyl 2,6-bis(bromomethyl)benzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with diphenylmethyl hydroxyisophthalate)

RN 113585-50-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 131 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:186795 CAPLUS

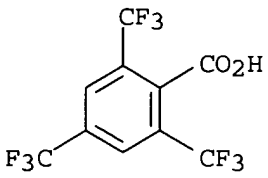
DN 108:186795

TI Polyfluoroaryl organometallic compounds. XVII. 2,4,6-Tris(trifluoromethyl)phenyllithium, a sterically crowded system

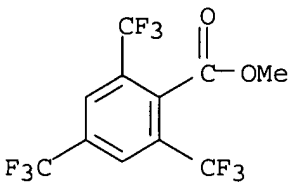
AU Carr, G. E.; Chambers, R. D.; Holmes, T. F.; Parker, D. G.

10803578

CS Sci. Lab., Univ. Durham, Durham, DH1 3LE, UK
SO Journal of Organometallic Chemistry (1987), 325(1-2), 13-23
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
OS CASREACT 108:186795
AB Reaction of 1,3,5-(HO2C)3C6H3 with SF4 at 150° yields 33% 1,3,5-(F3C)3C6H3 (I). The lithium derivative 1,3,5-(F3C)3C6H2Li (II) generated from I with BuLi in hexane-Et2O is remarkably thermally stable. I is less acidic than pentafluorobenzene in competition for BuLi. A variety of derivs. of II were prepared from common reagents in spite of crowding in the system, including the products [1,3,5-(F3C)3C6H2]2Hg and 1,3,5-(F3C)3C6H2R (R = Cl, Br, SH, SO2Li, CO2H, CO2Me, COCO2H, SiMe3, SnMe3, etc.).
IT **25753-26-8P**, 2,4,6-Tris(trifluoromethyl)benzoic acid
114071-23-7P, Methyl 2,4,6-tris(trifluoromethyl)benzoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 25753-26-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 114071-23-7 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



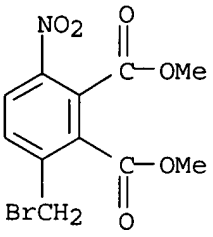
L3 ANSWER 132 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:168061 CAPLUS
DN 108:168061
TI Synthesis and chemiluminescence of copolymers of 5-amino-8-vinyl-phthalazine-1,4(2H,3H)-dione with methyl methacrylate or styrene, and of α,ω-bis[5-amino-phthalazine-1,4(2H,3H)-dion-]8-yl alkanes [=α,ω-bis(6-luminyl)alkanes]: investigations on an intramolecular 'distance effect'
AU Gundermann, Karl Dietrich; Lieske, Dieter; Haase, Brigitte; Hartmann-Azanza Baca, Brigitte
CS Inst. Org. Chem., Tech. Univ. Clausthal, Clausthal-Zellerfeld, D-3392, Fed. Rep. Ger.
SO Journal of Bioluminescence and Chemiluminescence (1987), 1(4), 201-13
CODEN: JBCHE7; ISSN: 0884-3996
DT Journal
LA English
AB Oligomers of 5-amino-8-vinylphthalazine-1,4(2H,3H)-dione (I) exhibited

about 0.05% of the chemiluminescence quantum yield of the corresponding monomer unit, i.e., 5-amino-8-ethylphthalazine-1,4(2H,3H)-dione which has a similar quantum yield to luminol. The quantum yields of copolymers of I with Me methacrylate or with styrene increased ≤1000-fold, relative to the quantum yield of oligomers of I. Thus the monomer units of Me methacrylate or styrene acted as spacers between the lumigenic groups. α,ω-Bis[(5-aminophthalazine-1,4(2H,3H)-dion)-8-yl]alkanes showed an analogous distance effect: the chemiluminescence quantum yield increased with increasing alkane chain length.

IT **71634-30-5**, Dimethyl 3-bromomethyl-6-nitrophthalate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triphenylphosphine)

RN 71634-30-5 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-6-nitro-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 133 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:123735 CAPLUS

DN 108:123735

TI Cyclic polyether compounds

IN Sakaki, Toru; Ogata, Takayuki; Yanagi, Hiroyuki; Nishida, Haruo

PA Tokuyama Soda Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAF

DT Patent

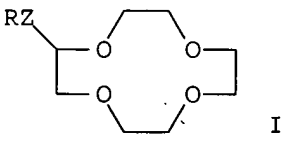
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62033170	A2	19870213	JP 1985-172287	19850807
	JP 03027551	B4	19910416		
PRAI	JP 1985-172287		19850807		

OS CASREACT 108:123735

GI



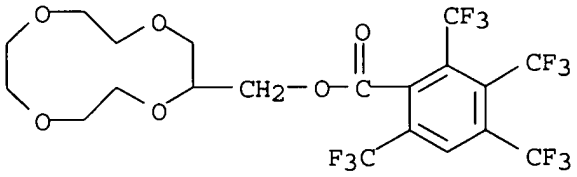
I

AB The title compds. [I; R = aryl; Z = (CH2)lCH2OCH2, (CH2)lCO2CH2, O(CH2)l+1CH2OCH2, O(CH2)lCH2CO2CH2, CONHCH2(CH2)lCO2CH2; l = 0-7] were prepared I are highly selective toward Na+ and thereby are useful for Na ion selective electrodes. Thus, a mixture of 5 mmol I (RZ = HOCH2), 5 mmol

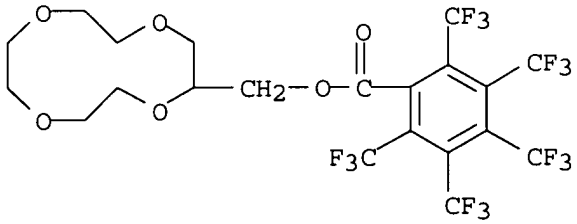
p-(chloromethyl)biphenyl; and 5 mmol NaOH in Me2CO was refluxed for 96 h to give 42% I (RZ = QCH2OCH2; Q = p-biphenyl). Electrodes made from .apprx.100 μ polyvinyl film containing I and p-nitrophenyl octyl ether show 10-60 times greater selectivity toward Na than K ion.

IT **109108-10-3P 109108-11-4P**
RL: DEV (Device component use); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of, for sodium ion selective electrode)

RN 109108-10-3 CAPLUS
CN Benzoic acid, 2,3,4,6-tetrakis(trifluoromethyl)-, 1,4,7,10-tetraoxacyclododec-2-ylmethyl ester (9CI) (CA INDEX NAME)



RN 109108-11-4 CAPLUS
CN Benzoic acid, pentakis(trifluoromethyl)-, 1,4,7,10-tetraoxacyclododec-2-ylmethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 134 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:497844 CAPLUS
DN 107:97844
TI Cyclic polyether-modified thermoplastic resins
IN Sakaki, Toru; Ogata, Takayuki; Horimoto, Hikari; Tsubaki, Shigeko
PA Tokuyama Soda Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 95 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

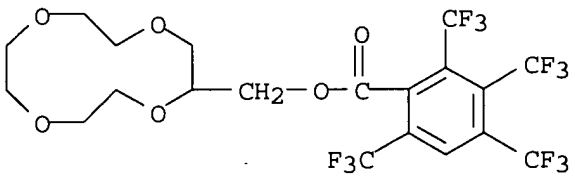
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62070452	A2	19870331	JP 1985-210179	19850925
	JP 01024824	B4	19890515		
PRAI	JP 1985-210179		19850925		

AB Mixts. of a thermoplastic resin and 0.1-40.0 phr 12-crown-4 derivative containing a group such as R(CH2)nOCH2 (n = 1-4), R(CH2)sCO2CH2 (s = 0-3), RO(CH2)mOCH2 (m = 2-6), RO(CH2)qCO2CH2 (q = 1-3), or RCONH(CH2)tCO2CH2 (t = 1-3) [R = aromatic group such as biphenyl-4-yl, anthryl, phenanthryl, p-phenylazophenyl, anthraquinonyl, pyrenyl, fluorenyl, p-styrylphenyl, bis-, tris-, or tetrakis(trifluoromethyl)phenyl, tri-, tetra-, or pentahalophenyl, or p-(p-alkoxyphenylazo)phenyl)] are useful for preparing

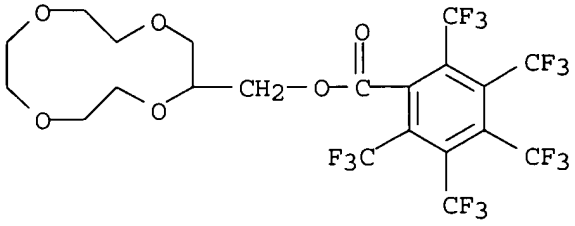
electrodes which have good Na+ selectivity and sensitivity and are suitable for removing or concentrating Na salts, etc. A mixture of p-(chloromethyl)biphenyl 5, (hydroxymethyl)-12-crown-4 5, and KOH 5 mmol in acetone was refluxed 96 h to give [(biphenyl-4-ylmethoxy)methyl]-12-crown-4 which (20 mg) was mixed with 200 mg PVC, 400 mg o-nitrophenyl octyl ether, and 10 mL THF and cast on glass to give a membrane (.apprx.100 μ) having Na selectivity ratio 20.

IT **109108-10-3 109108-11-4**
RL: TEM (Technical or engineered material use); USES (Uses)
(thermoplastics containing, for electrodes with sodium ion sensitivity)

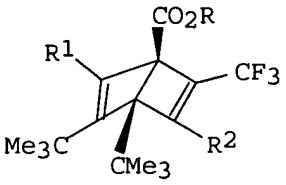
RN 109108-10-3 CAPLUS
CN Benzoic acid, 2,3,4,6-tetrakis(trifluoromethyl)-, 1,4,7,10-tetraoxacyclododec-2-ylmethyl ester (9CI) (CA INDEX NAME)



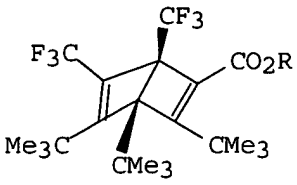
RN 109108-11-4 CAPLUS
CN Benzoic acid, pentakis(trifluoromethyl)-, 1,4,7,10-tetraoxacyclododec-2-ylmethyl ester (9CI) (CA INDEX NAME)



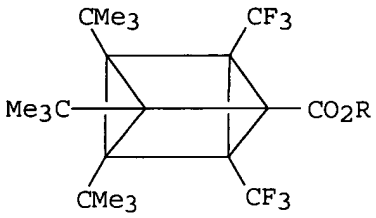
L3 ANSWER 135 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:213474 CAPLUS
DN 106:213474
TI Syntheses with cyclobutadienes. 15. Prismane-Dewar benzene isomerization - x-ray crystal structure of tert-butyl 3,4,5-tri-tert-butyl-2,6-bis(trifluoromethyl)prismane-1-carboxylate
AU Wingert, Horst; Maas, Gerhard; Regitz, Manfred
CS Fachbereich Chem., Univ. Kaiserslautern, Kaiserslautern, D-6750, Fed. Rep. Ger.
SO Tetrahedron (1986), 42(19), 5341-53
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 106:213474
GI



I



II



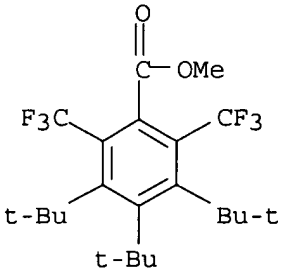
III

AB Substituted Dewar benzene derivs. I (R, R1 = CMe3; R2 = CF3) and II (R = CMe3) yield the corresponding acids by loss of CH2:CMe2 when heated to 150-200°; isomerization to the benzoic acid does not occur. Prismane derivative III (R = CMe3), which is obtained from II (R = CMe3) photochem., also loses CH2:CMe2 at 150°, but II (R = H) rearranges to the isomeric I (R = H; R1 = CF3; R2 = CMe3) and II (R = H) on prolonged heating at 150°. I (R = Me; R1 = CF3; R2 = CMe3) and II (R = Me) are converted into III (R = Me) photochem. The crystal structure of II (R = CMe3) is reported.

IT **108312-87-4P 108312-94-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(attempted preparation of)

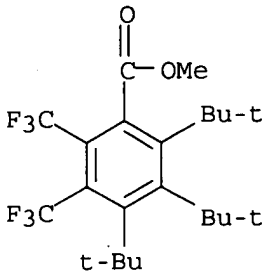
RN 108312-87-4 CAPLUS

CN Benzoic acid, 3,4,5-tris(1,1-dimethylethyl)-2,6-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

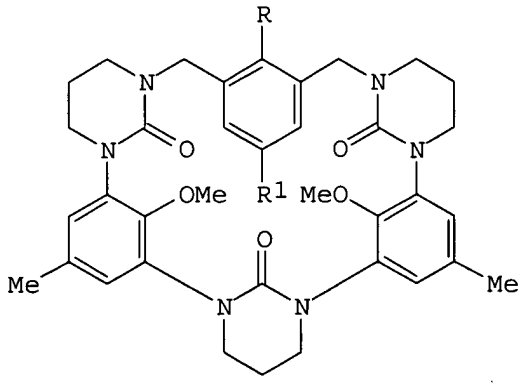


RN 108312-94-3 CAPLUS

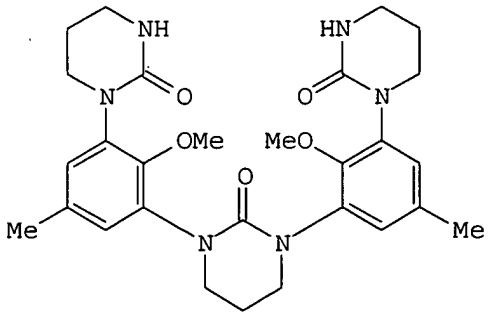
CN Benzoic acid, 2,3,4-tris(1,1-dimethylethyl)-5,6-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



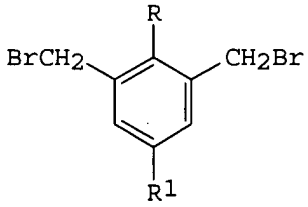
L3 ANSWER 136 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:32979 CAPLUS
DN 106:32979
TI Host-guest complexation. 40. Synthesis and complexation of macrocyclic hosts containing cyclic ureas, anisyls, and steric barriers
AU Stewart, Kent D.; Miesch, Michel; Knobler, Carolyn B.; Maverick, Emily F.; Cram, Donald J.
CS Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024, USA
SO Journal of Organic Chemistry (1986), 51(23), 4327-37
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 106:32979
GI



I



II

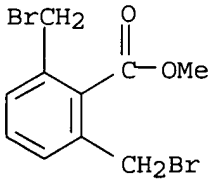


III

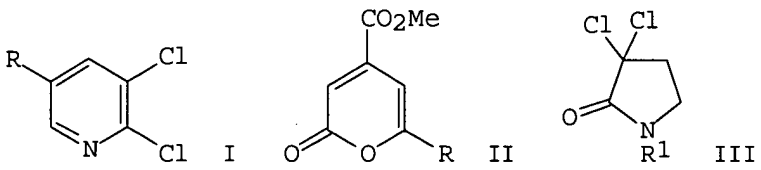
AB Eight macrocyclic hosts I (R = H, Br, 3,5-di-tert-butyl-4-methoxyphenyl, R1 = H, CMe3; R = CO2Me, 9-anthracenyl, R1 = H) were prepared by cyclizing pyrimidone II with the appropriate m-bis(bromomethyl)benzene derivs. III in THF containing NaH. The association consts. and free energies of complexation

of I with alkali metal cations and ammonium and alkylammonium ions in COCl3 saturated with H2O were determined by the extraction method. Substitution of H in the R position of I (R = R1 = H) with Br or CO2Me decreased the binding of alkali metal cations by 0-2 kcal/mol. Incorporation of steric barriers into the bridging m-xylylene units provides host which discriminate in binding MeNH3+ and Me3CNH3+ by ≥2.5 kcal/mol.

IT **56263-51-5P**, Methyl 2,6-bis(bromomethyl)benzoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 137 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1986:533716 CAPLUS
DN 105:133716
TI Metal-catalyzed additions of organic polyhalides to olefins. 4. Convenient approaches to heterocycles via copper-catalyzed additions of organic polyhalides to activated olefins
AU Martin, Pierre; Steiner, Eginhard; Streith, Jacques; Winkler, Tammo; Bellus, Daniel
CS Cent. Funct. Res., CIBA-GEIGY A.-G., Basel, CH-4002, Switz.
SO Tetrahedron (1985), 41(19), 4057-78
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 105:133716
GI



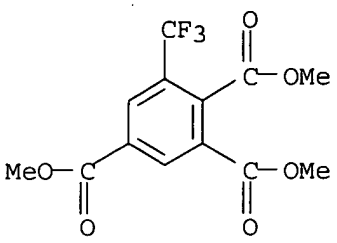
AB An efficient one-pot method for the synthesis of 2,3-dichloro-5-substituted pyridines I [R = Cl, Me, CF3, Et, Pr, Bu, CHMe2, Me(CH2)4, CH2CH2Cl, CH2CHCl2, CH2CCl3] starting from the 1:1 adducts of the Cu-catalyzed addition of RCCl2CHO to H2C:CHCN is presented. Similarly, the CuCl-catalyzed reaction of Me itaconate with RCCl3 gives 2-pyrones II (R = Cl, CF3, CO2Me) via dehalogenation and subsequent thermal ring closure of the primary 1:1-adducts. The new electrophilic 2-pyrone II (R = CF3) undergoes [4+2]-cycloaddn. reactions with inverse electron demand with olefins and acetylenes, allowing regioselective transfer of a group from CCl3CF3 into more complex organic mols. The 1:1-adduct of CCl3COCl with Me

acrylate gave novel N-substituted derivs. III (R1 = H, CHMe2, Ph, substituted Ph, NHCO2Et) of pyroglutamic acid as well as of proline.

IT **101640-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 101640-72-6 CAPLUS

CN 1,2,4-Benzenetricarboxylic acid, 6-(trifluoromethyl)-, trimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 138 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:461096 CAPLUS

DN 105:61096

TI Supported catalysts for polymerization of olefins

IN Johnson, Bryce V.; Karayannis, Nicholas M.; Hoppin, Charles R.; Ornellas, Linda

PA Amoco Corp., USA

SO U.S., 11 pp.
CODEN: USXXAM

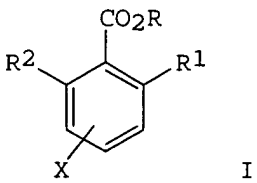
DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4581342	A	19860408	US 1984-674996	19841126
	CA 1253134	A1	19890425	CA 1985-495883	19851121
	EP 187462	A2	19860716	EP 1985-308543	19851125
	EP 187462	A3	19880518		
	EP 187462	B1	19900425		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AT 52264	E	19900515	AT 1985-308543	19851125
	JP 61136508	A2	19860624	JP 1985-265979	19851126
	US 4657882	A	19870414	US 1985-813603	19851226
PRAI	US 1984-674996	A	19841126		
	EP 1985-308543	A	19851125		

GI



I

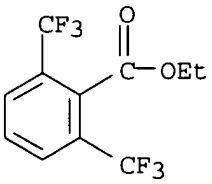
AB The title catalysts, giving good stereospecificity and morphol., are prepared by complexing Mg alkyls with the esters I (R = C1-10 alkyl; R1, R2 = C1-6 alkyl, Cl, Br; X = H, alkyl, aryl, OR, or halogen), treating the

products with precipitants, and reaction of the solid with Ti(IV) compds. and electron donors. Thus, adding 3.75 mL Et 2,4,6-trimethylbenzoate to 75 mL solution of 10.3% Bu2Mg and Et3Al in hexane gave a complex which was added over 45 min to 75 mL SiCl4 and heated for 16 h at 40° to precipitate a white solid containing Cl 43.9, Mg 14.9, and I 32.1%. A mixture of this solid 3.6, TiCl4 18.2, diiso-Bu phthalate 1.6 g and 100 mL PhMe was refluxed for 2 h, combined with 75 mL PhMe, heated at 108° for 30 min, decanted, added to 100 mL TiCl4, and heated at 110° for 1 h to give a solid containing Cl 54.1, Mg 13.8, Ti 4.31, phthalate 21.4, and I 0.4%. C3H6 was polymerized at 160° F/250 psig in the presence of 20 mg this solid and Et3Al (Al-Ti >200:1) for 2 h to give 5963 g polypropylene/g Ti component, bulk d. 23.0 lbs/ft3, containing 1.6% extractables.

IT **38570-08-0D**, reaction products with magnesium alkyls, halides, titanium compds. and electron donors
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for polymerization of olefins)

RN 38570-08-0 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 139 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1986:168314 CAPLUS

DN 104:168314

TI Metal-catalyzed additions of organic polyhalides to olefins. Part 3. A new electrophilic 2-pyrone bearing a trifluoromethyl group, its preparation and its [4 + 2] cycloaddition reactions

AU Martin, Pierre; Streith, Jacques; Rihs, Grety; Winkler, Tammo; Bellus, Daniel

CS Ciba-Geigy A.-G., Basel, CH-4002, Switz.

SO Tetrahedron Letters (1985), 26(33), 3947-50
CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 104:168314

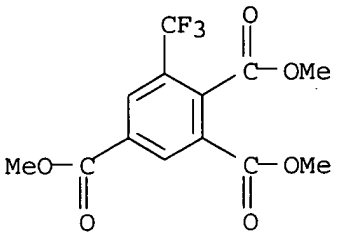
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Trifluoromethyl-2H-pyran-2-one I was prepared starting from the 1:1-adduct F3CCCl2CH2CCl(CO2Me)CH2CO2Me of the CuCl-catalyzed addition of F3CCCl3 to di-Me itaconate. I affords [4 + 2] cycloadducts with a number of olefins and acetylenes. Thus, I and 4-ClC6H4C.tplbond.CCl and indene gave bicyclic compds. II and III, resp. Their formation follows the reactivity patterns of a typical Diels-Alder reaction with inverse electron demand. The overall sequence represents a new methodol. for the transfer of the CF3-group from a simple Freon into more complex organic compds. The mol. structure of II was determined by x-ray crystal structure anal.

10803578

IT **101640-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 101640-72-6 CAPLUS
CN 1,2,4-Benzenetricarboxylic acid, 6-(trifluoromethyl)-, trimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 140 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1986:83798 CAPLUS
DN 104:83798
TI Herbicidal sulfonamides
IN Pasteris, Robert James; Thompson, Mark Ewell; Wexler, Barry Arthur
PA du Pont de Nemours, E. I., and Co. , USA
SO Eur. Pat. Appl., 71 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 155767	A1	19850925	EP 1985-301119	19850220
	EP 155767	B1	19900816		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	US 4609397	A	19860902	US 1984-679145	19841211
	US 4609395	A	19860902	US 1984-686796	19841226
	AU 8538797	A1	19850912	AU 1985-38797	19850218
	AU 570298	B2	19880310		
	CA 1221693	A1	19870512	CA 1985-474642	19850219
	CA 1221694	A1	19870512	CA 1985-474643	19850219
	JP 60214780	A2	19851028	JP 1985-30672	19850220
	JP 03079349	B4	19911218		
	EP 333304	A2	19890920	EP 1989-200910	19850220
	EP 333304	A3	19900725		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 60222466	A2	19851107	JP 1985-39009	19850301
	US 4693743	A	19870915	US 1986-863606	19860515
	US 4746355	A	19880524	US 1986-886151	19860716
	US 4853025	A	19890801	US 1988-156007	19880216
PRAI	US 1984-581817	A	19840221		
	US 1984-585170	A	19840301		
	US 1984-679145	A	19841211		
	US 1984-686796	A	19841226		
	EP 1985-301119	P	19850220		
	US 1986-886151	A3	19860716		

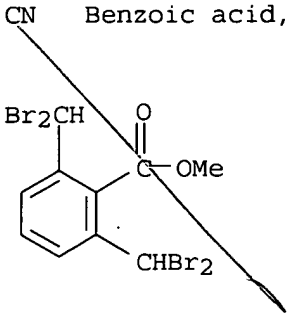
OS CASREACT 104:83798
AB The heterocyclic sulfonamides RSO2NHCONR1R2 (R = substituted pyrazolyl, imidazolyl, thienyl, pyridyl, benzofuranyl, etc.; R1 = H, Me; R2 = pyrimidyl, triazinyl, etc.) are herbicides. Thus, pre-emergence application of Et 5-[[[[4,6-dimethoxypyrimidin-2-

yl]aminocarbonyl]aminosulfonyl]methyl]-1,3-dimethyl-1H-pyrazole-4-carboxylate (2 kg/ha) totally controlled nutsedge (Cyperus rotundus), in pot expts. The compds. can be prepared by reacting a sulfonyl isocyanate RSO2NCO with an appropriate heterocyclic amine HNR1R2.

IT **100555-58-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 100555-58-6 CAPLUS

CN Benzoic acid, 2,6-bis(dibromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 141 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1985:525168 CAPLUS

DN 103:125168

TI Fluorine-containing polyamide acid derivative and polyimide

IN Numata, Shunichi; Fujisaki, Koji; Kinjo, Noriyuki

PA Hitachi, Ltd. , Japan; Hitachi Chemical Co., Ltd.

SO Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW

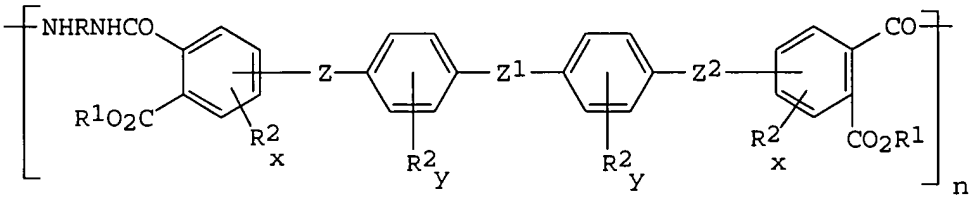
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 142149	A2	19850522	EP 1984-113629	19841112
	EP 142149	A3	19870304		
	EP 142149	B1	19950201		
	R: DE, FR, GB, NL				
	JP 60104129	A2	19850608	JP 1983-211075	19831111
	JP 02014366	B4	19900406		
	CN 85101150	A	19870117	CN 1985-101150	19850401
PRAI	JP 1983-211075	A	19831111		

GI



I

AB Polyamic acids I [Z, Z2 = O, CO2, or C(O)S; R2 = alkyl, fluorinated alkyl, or halogen; R = residue formed by removing 2 amino groups from a diamine; R1 = H or alkyl; Z1 = perfluoroalkylene; x = 0-3, y = 1-4] are prepared and converted to polyimides which have good heat resistance and low moisture absorption and are useful for protective films for semiconductor devices,

etc. The polyamic acids exhibit good soluble in polar solvents. Thus, 2.05 g p-phenylenediamine in 85 g N-methyl-2-pyrrolidone was treated at 20° with 12.95 g 2,2-bis[4-(3,4-dicarboxybenzoyloxy)phenyl]-1,1,1,3,3,3-hexafluoropropane and aged .apprx.5 h to prepare a varnish having viscosity 250 P. The varnish was coated on glass and heated at 150-400° to prepare a polyimide film which was not brittle and absorbed 0.75% water (25°, 75% relative humidity). Samples of the film lost 3% of their weight during 9, 21, 46, and 200 min at 500, 490, 475, and 450°, resp., in N. Other samples of the film lost 3% of their weight during 20, 85, 120, and 220 min at 475, 450, 440, and 425°, resp.

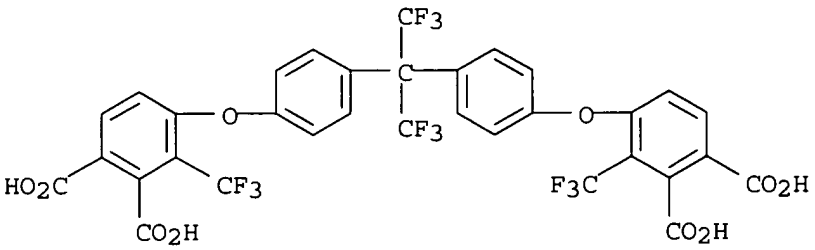
IT **98180-60-0P**
RL: TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(coatings, elec. insulating, heat- and water-resistant, preparation of)

RN 98180-60-0 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[3-(trifluoromethyl)-, polymer with 4,4'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis(4,1-phenyleneoxy)]bis[benzenamine] (9CI) (CA INDEX NAME)

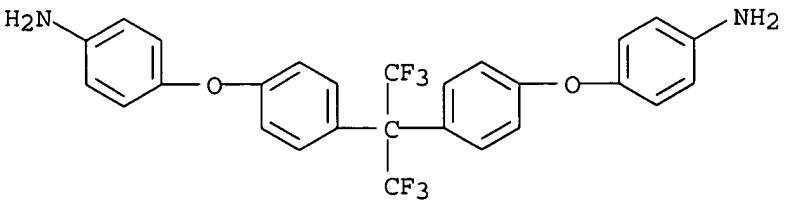
CM 1

CRN 98180-59-7
CMF C33 H16 F12 O10



CM 2

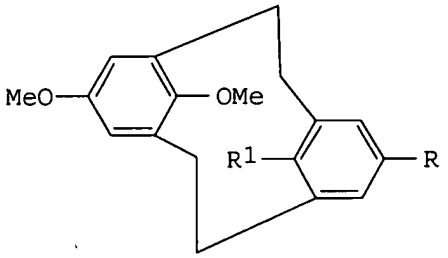
CRN 69563-88-8
CMF C27 H20 F6 N2 O2



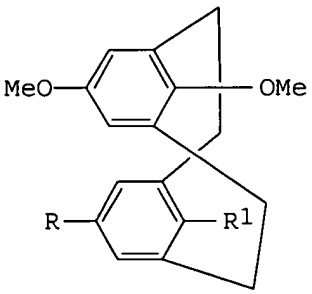
L3 ANSWER 142 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1985:220541 CAPLUS
DN 102:220541
TI Electron donor-acceptor compounds. XXXVIII. Electron donor-acceptor [2.2]metacyclophanes: synthesis, structure, and charge-transfer spectra
AU Staab, Heinz A.; Schanne, Lothar; Krieger, Claus; Taglieber, Volker

10803578

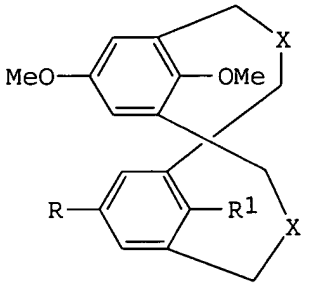
CS Abt. Org. Chem., Max-Planck-Inst. Med. Forsch., Heidelberg, D-6900, Fed. Rep. Ger.
SO Chemische Berichte (1985), 118(3), 1204-29
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 102:220541
GI



I



II



III

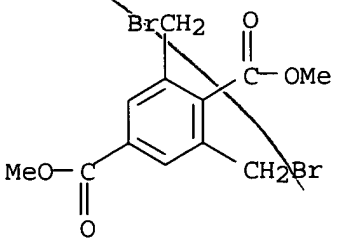
AB Donor-acceptor [2.2]metacyclophanes I and II (R = R1 = CO2Me, cyano) as well as I (R = NO2, R1 = H) were synthesized via the correspondingly substituted 2,11-dithia[3.3]metacyclophanes III (X = S) and their disulfone derivs. III (X = SO). The anti-compound I (R = R1 = CO2Me) and the syn-isomer II (R = R1 = CO2Me) were isolated and characterized. The attempt of the analogous synthesis of I and II (R = R1 = NO2) via III failed since with loss of the intraannular substituents and by transannular C-C formation a tetrahydropyrene derivative was formed. X-ray structure analyses of I (R = NO2, R1 = H) and III (X = S, R = NO2, R1 = H; R = R1 = NO2) were performed. The mol. structures of these compds. are related to steric strain and donor-acceptor overlap. The structure analyses confirm the assignment to the syn- and anti-series as derived from 1H NMR. Absorption spectra of I and II were measured; the surprising absorption behavior of the isomers I and II (R = R1 = CO2Me) with very different donor-acceptor overlap was of interest. Determination of the solvent dependence of fluorescence assured that the absorptions dealt with are indeed charge-transfer transitions.

IT **59346-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclization with dimethoxybenzenedimethanethiol)

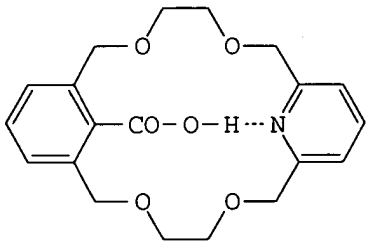
RN 59346-23-5 CAPLUS

CN 1,4-Benzenedicarboxylic acid, 2,6-bis(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

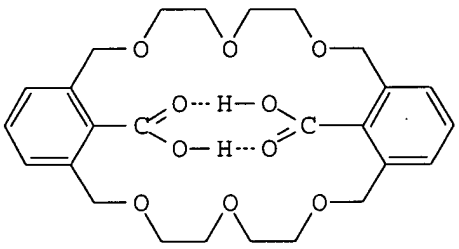
10803578



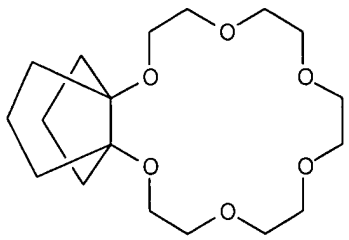
L3 ANSWER 143 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1982:527619 CAPLUS
DN 97:127619
TI Host-guest complexation. 24. Synthesis of multiheteromacrocycles containing intramolecularly interacting units or new steric barriers
AU Bell, Thomas W.; Cheng, Paul G.; Newcomb, Martin; Cram, Donald J.
CS Dep. Chem., Univ. California, Los Angeles, CA, 90024, USA
SO Journal of the American Chemical Society (1982), 104(19), 5185-8
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
GI



II



III

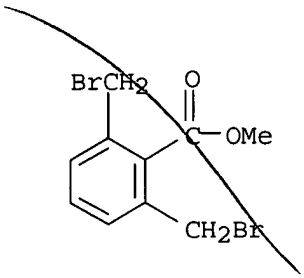


IV

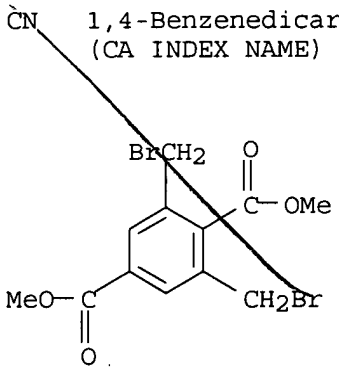
AB Six new multiheteromacrocyclic hosts containing 2,6-pyridinediyldimethylene (P), 2-carboxy-1,3-xylyl (A), 2-carbomethoxy-1,3-xylyl (M), 2,5-bis(carbomethoxy)-1,3-xylyl (T), 1,5-bicyclo[3.3.0]octanediyl (B), dimethylene (E), or oxygen (O) units are reported. Treatment of 2,6-bis[(2-hydroxyethoxy)methyl]pyridine [P(OEOH)2] with Me 2,6-bis(bromomethyl)benzoate (I) in THF-NaH gave 43% M(OEO)2P, hydrolysis of which gave A(OEO)2P (II), whose pyridine N and carboxylic H form a strong transannular H bond (pKa and crystal structure). The reaction of I with diethylene glycol (HOEOEOH) in THF-NaH gave 21% M(OEOEO)2M, which was hydrolyzed to A(OEOEO)2A (III), whose transannularly located carboxyl groups form a planar 8-membered ring containing linear hydroxyl-to-carbonyl H bonds (crystal structure and pKa). Similarly, T(OEOEO)2T was formed from TBr2 and HOEOEOH (18%). Treatment of B(OH)2 with (TsOEOEO)2E in THF-NaH

gave 25% B(OEOEO)2E (IV), whose ability to complex tert-butylammonium thiocyanate in CHCl3 saturated with H2O was only slightly less than that of E(OEOEO)2E.

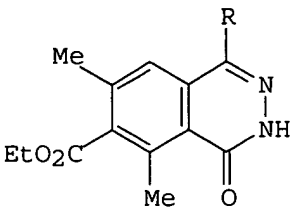
IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization reactions of)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



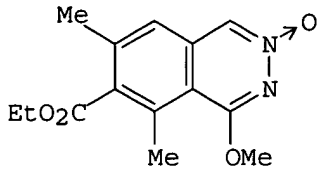
IT **59346-23-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with diethylene glycol)
RN 59346-23-5 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,6-bis(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



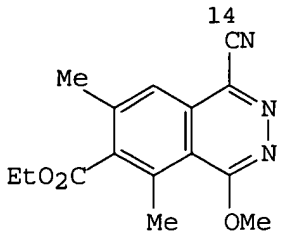
L3 ANSWER 144 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1982:52253 CAPLUS
DN 96:52253
TI Preparation of 1-[14C]-hydroxymethyl-6-ethoxycarbonyl-5,7-dimethyl-4-phthalazone (EG-626)
AU Abuki, Hideo; Miyazaki, Hiroshi
CS Pharm. Div., Nippon Kayaku Co., Tokyo, 115, Japan
SO Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(6), 889-96
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
OS CASREACT 96:52253
GI



I



II



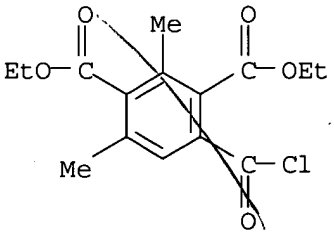
III

AB The title compound I (R = 14CH2OH) was prepared (sp. activity 33.64 μCi/mg) from 3,5-Me2C6H(CO2Et)3-1,2,4 in 11 steps, the key steps being the cyclocondensation reaction of 3,5,1-Me2(HCO)C6H(CO2Et)2-2,4 with NH2NH2.H2O to give the phthalazone I (R = H) and the Reissert-Henze reaction of the oxide II with K14CN to give the nitrile III.

IT **80523-71-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in carbon-14-labeled EG 626 preparation)

RN 80523-71-3 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 4-(chlorocarbonyl)-2,6-dimethyl-, diethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 145 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1981:45498 CAPLUS

DN 94:45498

TI Synthesis of (trifluoromethyl)phthalic acids

AU Hosokawa, Kenzo; Fujii, Shozo; Inukai, Kan

CS Gov. Ind. Res. Inst., Nagoya, 462, Japan

SO Nippon Kagaku Kaishi (1980), (8), 1304-6
CODEN: NKAKB8; ISSN: 0369-4577

DT Journal

LA Japanese

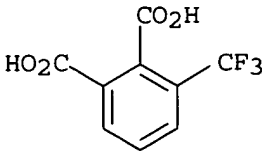
OS CASREACT 94:45498

AB The oxidation of (trifluoromethyl)naphthalenes (I) with CrO3 in AcOH was examined for the synthesis of (trifluoromethyl)phthalic acids (II). I generally underwent cleavage of the ring having no trifluoromethyl group, and the resulting II were isolated in 14.apprx.63% yields. However, 4-methoxy-1-(trifluoromethyl)naphthalene gave 3-(trifluoromethyl)phthalide together with 3-(trifluoromethyl)-3-hydroxyphthalide, and 5-nitro-1-(trifluoromethyl)naphthalene remained intact under these

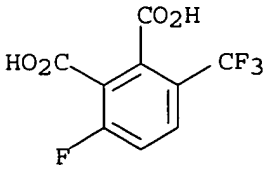
conditions.

IT **24913-62-0P 76284-56-5P 76284-57-6P**
76284-58-7P 76284-59-8P 76284-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

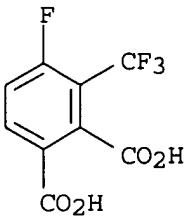
RN 24913-62-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



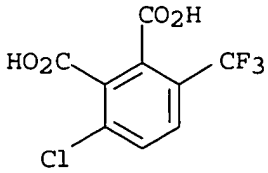
RN 76284-56-5 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-fluoro-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 76284-57-6 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-fluoro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

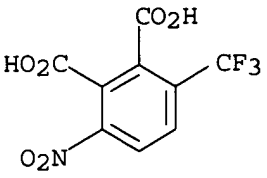


RN 76284-58-7 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-chloro-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

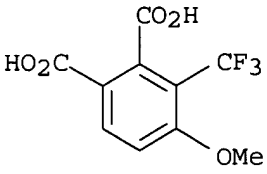


RN 76284-59-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-nitro-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10803578



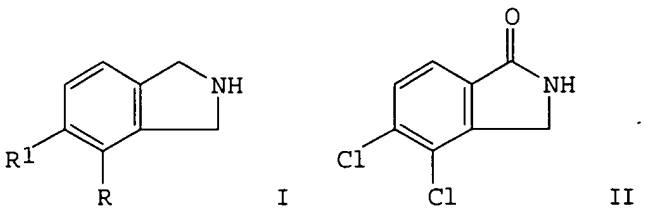
RN 76284-61-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 146 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1980:620588 CAPLUS
DN 93:220588
TI 4- and 5-Substituted 2,3-dihydro-1H-isoindoles, pharmaceutical compositions and method of inhibiting phenylethanolamine N-methyltransferase
IN Bondinell, William E.; Pendleton, Robert G.
PA Smithkline Corp., USA
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4218464	A	19800819	US 1979-17005	19790302
PRAI	US 1979-17005	A	19790302		

GI

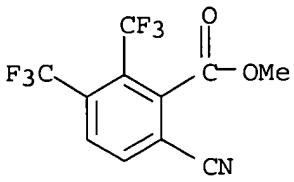


I II

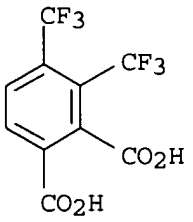
AB Dihydroisoindoles I (R, R1 = Cl, Br, F, iodo, CF3) were prepared Thus, 2,3-MeClC6H3NH2 was acetylated, chlorinated and hydrolyzed to give 2,3,4-MeCl2C6H2NH2, which was diazotized and converted via the nitrile to 2,3,4-MeCl2C6H2CO2H. The acid was esterified, treated with N-bromosuccinimide and then with NH3 to give dihydroisoindolone II, which was then reduced with B2H6 to I (R = R1 = Cl). I (R = R1 = Cl) caused 98% inhibition of phenylethanolamine N-methyltransferase at 1 + 10-4M in vitro.

10803578

IT **75571-05-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 75571-05-0 CAPLUS
CN Benzoic acid, 6-cyano-2,3-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

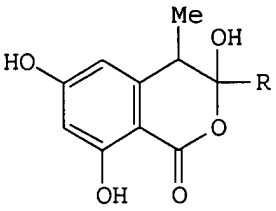


IT **75571-06-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 75571-06-1 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,4-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

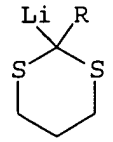


L3 ANSWER 147 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1980:446328 CAPLUS
DN 93:46328
TI Acetogenin synthesis. Organocopper reagents, anions of 1,3-dithianes and of protected cyanohydrins as intermediates in ketide side-chain synthesis
AU Colombo, Lino; Gennari, Cesare; Santandrea, Marco; Narisano, Enrica; Scolastico, Carlo
CS Ist. Chim. Org., Univ. Milano, Milan, 20133, Italy
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (1), 136-40
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 93:46328
GI

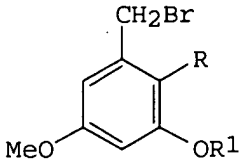
10803578



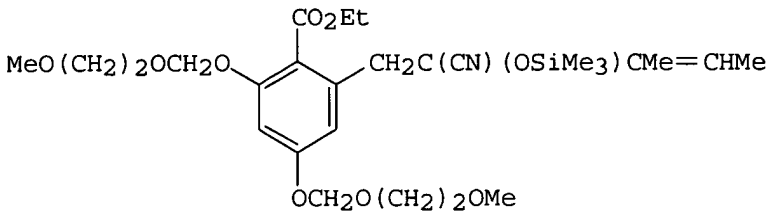
I



IV



V



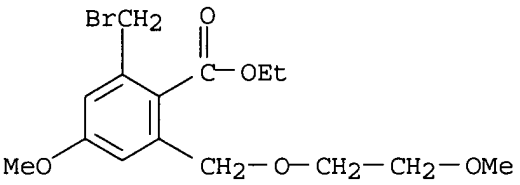
VI

AB The dihydroisocoumarins I (R = sec-Bu, CMe:CHMe) (II and III resp.) were prepared by reaction of the dithianes IV (R as before) with the bromides V [R = H, R1 = Me; R = CO2Et, R1 = CH2O(CH2)2OMe, resp.], followed by deprotection and cyclization. II was also prepared (86-90%) in 5 steps from 3,5-(MeO)2C6H3CH2COCl. A higher yield of III (82%) was obtained using the silylcyano intermediate VI derived in 3 steps from V [R = CO2Et, R1 = CH2O(CH2)2OMe] followed by deprotection and cyclization.

IT **74149-59-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation reaction of, with lithiomethylpropenyldithiane)

RN 74149-59-0 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-4-methoxy-6-[(2-methoxyethoxy)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 148 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1980:41891 CAPLUS

DN 92:41891

TI Pyridazino [3,4,5-de] phthalazines. I. Synthesis of the heterocyclic system and key intermediates

AU Francis, John E.; Doebel, Karl J.; Schutte, Paula M.; Savarese, Edgar C.; Hopkins, Stephen E.; Bachmann, Ernst F.

CS Res. Dep., Ciba-Geigy Corp., Ardsley, NY, 10502, USA

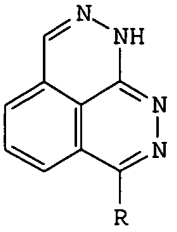
SO Canadian Journal of Chemistry (1979), 57(24), 3320-31
CODEN: CJCHAG; ISSN: 0008-4042

DT Journal

LA English

OS CASREACT 92:41891

GI



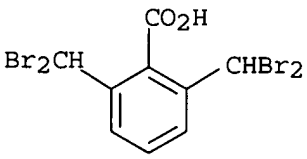
I

AB 1H-Pyridazino[3,4,5-de]phthalazine (I, R = H) and 3-hydrazino-1(or 9)H-pyridazino[3,4,5-de]phthalazine (I, R = NHNH2) represent intramol. hydrazones of the drugs hydralazine and dihydralazine, resp. These novel heterocycles were synthesized by several different routes starting from 2,6-dimethylbenzoic acid, 3-methylphthalic anhydride, or hemimellitic acid. Tetrabromination of 2,6-dimethylbenzoic acid with Br2 in CCl4 under free radical conditions followed by treatment with dilute aqueous N2H4.H2O produced pure I (R = H) in yields up to 58%. Treatment of 3-methylphthalic anhydride with 2 mol of N-bromosuccinimide under radical conditions followed by reaction of the dibromo compound with N2H4.H2O in Me Cellosolve produced 3-oxo-3H-2,9(or 3)-dihydropyridazino[3,4,5-de]phthalazine in 60% yield. This intermediate was converted to the 3-thiono compound or 3-chloro-1(or 9)H-pyridazino[3,4,5-de]phthalazine from which the hydrazine I (R = NHNH2) was generated by N2H4.H2O treatment. This hydrazine was further characterized by conversion with acid chlorides to novel tetracyclic condensed triazoles or by nitrous acid to a tetracyclic condensed tetrazole. I (R = H) was uninteresting in pharmacol. screens but the hydrazine I (R = NHNH2) resembled hydralazine by lowering blood pressure in several animal test models and in limited clin. trials.

IT **14346-75-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 14346-75-9 CAPLUS

CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)

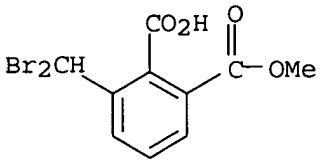


IT **14346-58-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with hydrazine)

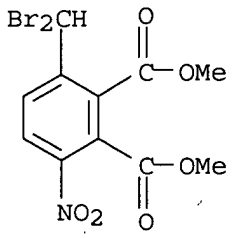
RN 14346-58-8 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3-(dibromomethyl)-, 1-methyl ester (9CI) (CA INDEX NAME)

10803578

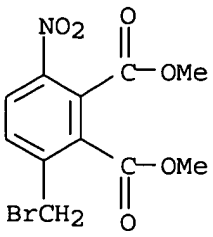


L3 ANSWER 149 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1979:593859 CAPLUS
DN 91:193859
TI Constitution and chemiluminescence. XI. Oligomers of 5-amino-8-vinylphthalazine-1,4(2H,3H)-dione
AU Gundermann, Karl Dietrich; Giesecke, Heinz
CS Org.-Chem. Inst., Tech. Univ. Clausthal, Clausthal-Zellerfeld, D-3392, Fed. Rep. Ger.
SO Liebigs Annalen der Chemie (1979), (8), 1085-93
CODEN: LACHDL; ISSN: 0170-2041
DT Journal
LA German
AB Di-Me 3-amino-6-vinylphthalate (I) [71616-03-0] was prepared by reaction of [(2,3-dicarbomethoxy-4-nitrophenyl)methyl]triphenylphosphonium bromide [71634-27-0] with bases and HCHO [50-00-0] and reduction of the resulting di-Me 3-nitro-6-vinylphthalate [71615-11-7]. Radical polymerization of I gave oligomers [71616-04-1] (average d.p. 15) which when treated with N2H4 produced a product (II) containing 5-aminophthalazinedione and N, 3-diaminophthalimide units. Hemin-catalyzed oxidation of II by aqueous alkaline H2O2 gave 0.05% of the chemiluminescence yield given by oxidation of luminol. This poor chemiluminescence efficiency of II may arise from neighboring group effects between chromophoric groups. At greater distances between luminol units, as in 8,8'-heptamethylenebis[5-aminophthalazine-1,4(2H,3H)-dione] [71634-28-1], the chemiluminescence yield is equal to that of luminol.
IT **71934-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71934-44-6 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(dibromomethyl)-6-nitro-, dimethyl ester (9CI) (CA INDEX NAME)

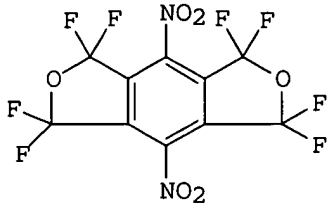


IT **71634-30-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triphenylphosphine)
RN 71634-30-5 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-6-nitro-, dimethyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 150 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1978:104804 CAPLUS
DN 88:104804
TI Derivatives of poly(trifluoromethyl)benzenes
AU Lukmanov, V. G.; Alekseeva, L. A.; Yagupol'skii, L. M.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1977), 13(10), 2129-35
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI



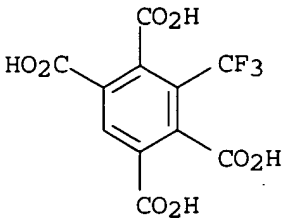
II

AB Treating 3,4,5- and 2,3,4-(HO2C)3C6H2NO2 and dinitropyromellitic acid with SF4 in anhydrous HF yielded 42% 3,4,5-(CF3)3C6H2NO2 (I), 13% 4-nitro-7-(trifluoromethyl)-1,1,3,3-tetrafluorophthalan and 41% benzodifuran II, resp. SnCl2 reduction of I yielded 93% 3,4,5-(CF3)3C6H2NH2(III), which was acetylated in refluxing Ac2O containing H2SO4. Diazotization and subsequent reaction of III gave 3,4,5-(CF3)3C6H2R [R = iodo, C6H2(CF3)3-3,4,5-N:NC6H4NMe2-p, N:NC6H3[N(CH2CH2OH)2]Me-4,2]. Brominating 1,2,3-(CF3)3C6H3 with KBr-SbF5 yielded 20% 2,3,4-and 40% 3,4,5-(CF3)3C6H2Br(IV) and 25% 2,3,4,5-Br(CF3)3C6HBr. Heating IV with CuCN gave 3,4,5-(CF3)3C6H2CN, which was hydrolyzed to the acid; the acid was also prepared by heating 1,2,3,5-(CF3)4C6H2 with SbS5 at 100° and then hydrolyzing. Treating (trifluoromethyl)pyromellitic acid with SF4-HF and then with aqueous NH3 afforded 50% C6H(CF3)5 and 3,2,4,6-R(CF3)3C6HCONH2 (IV; R = CF3, H2NCO) in 28 and 16% yield, resp. Treating IV with P2O5 and with KOBr gave the resp. nitriles and amines.

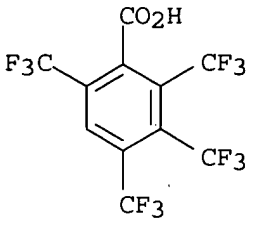
IT **53812-59-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination-amidation of)

RN 53812-59-2 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

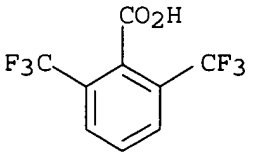
10803578



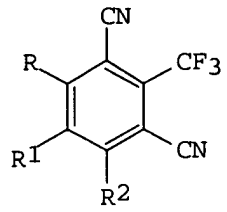
IT **65537-94-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and iodination of)
RN 65537-94-2 CAPLUS
CN Benzoic acid, 2,3,4,6-tetrakis(trifluoromethyl)- (9CI) (CA INDEX NAME)



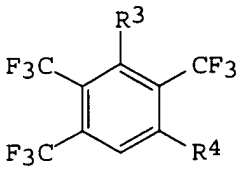
IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 151 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1978:62120 CAPLUS
DN 88:62120
TI Reaction of poly(trifluoromethylbenzenes) with liquid ammonia
AU Yagupol'skii, L. M.; Lukmanov, V. G.; Boiko, V. N.; Alekseeva, L. A.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1977), 13(11), 2388-91
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI



I, R=R2=H, R1=CN
II, R=H, R1=R2=CF3
III, R=R2=CF3 R1=CN



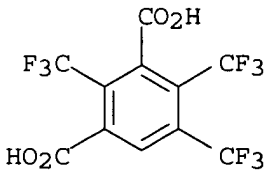
IV, R3=R4=CO2H
V, R3=COF, R4=CF3
VI, R3=CONH2, R4=CF3

AB Ammonolysis of tetrakis- (1,2,3,5), pentakis-, and hexakis(trifluoromethyl)benzene with liquid NH3 gave the resp. m-dinitriles I, II, and III. The nitriles were hydrolyzed to the acids by treatment with H2SO4-AcOH-H2O (1:1:1). Fluorination of diacid IV with SF4 gave monoacid fluoride V, which was converted into the amide VI with NH3.

IT **65387-31-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of, with sulfur tetrafluoride)

RN 65387-31-7 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 2,4,5-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 152 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:439151 CAPLUS

DN 87:39151

TI Optically active, aromatic spiranes, 5. Stereochemistry of metallocenes, 39. A universal method for the preparation, and determination of the absolute configuration and enantiomeric purity of chiral 2,2'-spirobiindanes

AU Meyer, Andre; Neudeck, Horst; Schloegl, Karl

CS Org.-Chem. Inst., Univ. Wien, Vienna, Austria

SO Chemische Berichte (1977), 110(4), 1403-20
CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

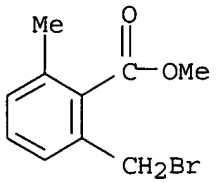
GI For diagram(s), see printed CA Issue.

AB (-)-Indanone Cr complexes I (R,R1 = H, Me, MeO) with phthalaldehydic esters II (R2,R3 = H, Me) and sequential treatment (hydrogenation, hydrolysis, cyclization, decomplexation, and hydrogenation) of the benzal derivs. gave chiral 2,2'-spirobiindans III. Chiralities and enantiomeric purities of the spirans can be deduced from those of I.

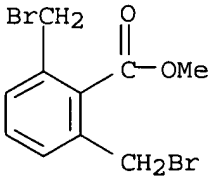
IT **56427-77-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

10803578

(Reactant or reagent)
(preparation and cyclization of)
RN 56427-77-1 CAPLUS
CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 153 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1977:139235 CAPLUS
DN 86:139235
TI Steric interactions of inner atoms in cyclic compounds. Part XXVII. The influence of exocyclic substituents on ring topomerizations
AU Foerster, Hans; Voegtle, Fritz
CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, Fed. Rep. Ger.
SO Journal of Chemical Research, Synopses (1977), (1), 30-1
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA French
GI For diagram(s), see printed CA Issue.
AB The activation parameters for ring topomerization in the metabenzenophanes I [R = Me, R1 = H, n = 7,8; R = OMe, R1 = H, n = 9 (II-IV); R = R1 = Me, R2 = H, Me, n = 7] were measured by nuclear magnetic double resonance line-shape anal. The effects of R2 in II-IV correlate with σR0 Hammett substituent consts., when R2 is electron-releasing the ring inversion is retarded whereas it is accelerated when R2 is electron-withdrawing. Very large R2 increase the topomerization threshold unexpectedly strongly whereas the exocyclic Me groups in I (R = R1 = Me, R2 = H, Me, n = 7) facilitate the topomerization; both phenomena are explained by buttressing effects. The anisochrony of the benzylic methylene protons in II-IV is strongly affected by R2; a σR0 dependence was found and its cause is discussed.
IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methoxylation of)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



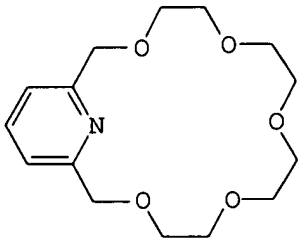
L3 ANSWER 154 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:446780 CAPLUS
DN 85:46780
TI Multiheteromacrocycles
IN Cram, Donald J.

10803578

PA University of California, USA
SO Ger. Offen., 144 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2539324	A1	19760325	DE 1975-2539324	19750904
	US 3965116	A	19760622	US 1974-505576	19740912
	GB 1481671	A	19770803	GB 1975-34582	19750820
	NL 7510478	A	19760316	NL 1975-10478	19750905
	FR 2285389	A1	19760416	FR 1975-27967	19750911
	JP 51125100	A2	19761101	JP 1975-111598	19750912
	FR 2300089	A1	19760903	FR 1976-16235	19760528
	FR 2300089	B1	19790727		
	US 4128556	A	19781205	US 1977-853445	19771121
PRAI	US 1974-505576	A	19740912		
	US 1976-662564	A3	19760301		

GI

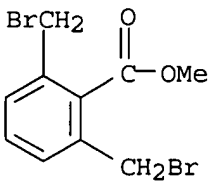


I

AB Crown ethers containing pyridine, furan, o-phenylene, or p-phenylene units were prepared and their complexing behavior investigated. Thus, I was obtained in 29% yield by treating 2,6-pyridinedimethanol with 4-MeC6H4SO2(OCH2CH2)4O3SC6H4Me-4. I formed a complex with Me3CNH3+SCN-, which had an association constant of 1.4 + 106 M-1 at 24°.

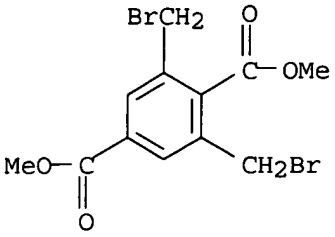
IT **56263-51-5P 59346-23-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with tetraethylene glycol)

RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 59346-23-5 CAPLUS
CN 1,4-Benzenedicarboxylic acid, 2,6-bis(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 155 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:446684 CAPLUS
DN 85:46684
TI 2,6-Disubstituted 2-phenyliminoimidazolidines and their acid addition salts
IN Staehle, Helmut; Koeppe, Herbert; Kummer, Werner; Hoefke, Wolfgang
PA Boehringer, C. H., Sohn, Fed. Rep. Ger.
SO Ger. Offen., 25 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2446758	A1	19760422	DE 1974-2446758	19741001
	DE 2446758	C3	19790104		
	AT 7507228	A	19771115	AT 1975-7228	19750922
	SU 575026	D	19770930	SU 1975-2174605	19750923
	DD 123602	C	19770105	DD 1975-188613	19750929
	CS 193524	P	19791031	CS 1975-6573	19750929
	BE 834051	A1	19760330	BE 1975-160578	19750930
	DK 7504418	A	19760402	DK 1975-4418	19750930
	FI 7502728	A	19760402	FI 1975-2728	19750930
	FI 61883	B	19820630		
	FI 61883	C	19821011		
	NO 7503314	A	19760402	NO 1975-3314	19750930
	NO 143459	B	19801110		
	NO 143459	C	19810218		
	NL 7511490	A	19760405	NL 1975-11490	19750930
	JP 51059863	A2	19760525	JP 1975-118196	19750930
	JP 60018653	B4	19850511		
	ZA 7506185	A	19770629	ZA 1975-6185	19750930
	ES 441385	A1	19770801	ES 1975-441385	19750930
	PL 97003	P	19780131	PL 1975-183670	19750930
	GB 1515019	A	19780621	GB 1975-40012	19750930
	PL 98984	P	19780630	PL 1975-197816	19750930
	CA 1056836	A1	19790619	CA 1975-236670	19750930
	IL 48214	A1	19791031	IL 1975-48214	19750930
	CH 620682	A	19801215	CH 1975-12678	19750930
	HU 20949	O	19810928	HU 1975-BO1573	19750930
	HU 178469	P	19820528		
	SE 7511028	A	19760402	SE 1975-11028	19751001
	SE 418497	B	19810609		
	SE 418497	C	19810917		
	FR 2286649	A1	19760430	FR 1975-30117	19751001
	FR 2286649	B1	19790914		
	JP 62010989	B4	19870310	JP 1976-674	19760101
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	ES 444901	A1	19770416	ES 1976-444901	19760204
	ES 444889	A1	19770516	ES 1976-444889	19760204

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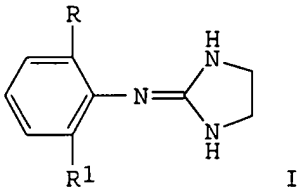
	ES 444898	A1	19770516	ES 1976-444898	19760204
	AT 7704211	A	19790315	AT 1977-4211	19770615
	AT 352717	B	19791010		
	AT 7704212	A	19790315	AT 1977-4212	19770615
	AT 352718	B	19791010		
	AT 7704213	A	19790415	AT 1977-4213	19770615
	AT 353265	B	19791112		
	AT 7704214	A	19790415	AT 1977-4214	19770615
	AT 353266	B	19791112		
	US 4125620	A	19781114	US 1977-850780	19771111
	CS 193550	P	19791031	CS 1978-4442	19780704
	CH 626352	A	19811113	CH 1980-5064	19800701
	CH 627452	A	19820115	CH 1980-5062	19800701
	CH 627453	A	19820115	CH 1980-5063	19800701
	CH 627454	A	19820115	CH 1980-5065	19800701
PRAI	DE 1974-2446758	A	19741001		
	AT 1975-7228	A	19750922		
	US 1975-615930	A2	19750923		
	CS 1975-6573	A3	19750929		
	CH 1975-12678	A	19750930		
	US 1976-720991	A2	19760907		

GI



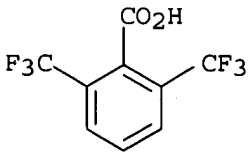
I

AB Antihypertensive (no data) phenyliminoimidazolidines I (R = R1 = F, OMe, OH, CF3; R = Me, R1 = Et, Br; R = Cl, R1 = F, Br, CF3) were prepared by condensing 2,6-RR1C6H3NHC(SMe):N+H2I- or 2,6-RR1C6H3N:CCl2 with H2NCH2CH2NH2.

IT **24821-22-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of)

RN 24821-22-5 CAPLUS

CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 156 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

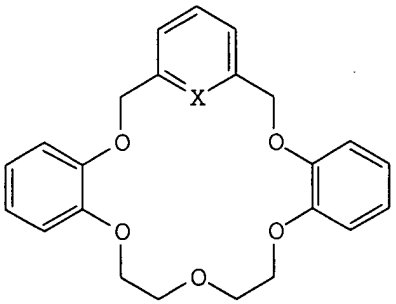
AN 1976:446618 CAPLUS

DN 85:46618

TI Ligand structure and complexation, V. New crown ethers and their alkali metal ion complexes

10803578

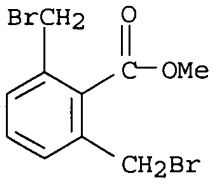
AU Weber, Edwin; Voegtle, Fritz
CS Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, Fed. Rep. Ger.
SO Chemische Berichte (1976), 109(5), 1803-31
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
GI



I

AB Neutral cyclic ligands, of varying ring size and flexibility, with the crown ether structure, e.g. I [X = N, N(O), CH, CF, COMe, CNO2, CS(O)Me], were prepared Chiral crown ethers were formed by incorporating sulfoxide functions or biphenyl moieties. Complexation and phase transfer properties were discussed as a function of ligand structure and stereochem. Changes in spectroscopic properties when the ligands were complexed with alkali metal, NH4+, heavy metal, and rare earth salts were studied. S and N analogs of I were also prepared

IT **56263-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization with trioxaundecanedithiol)
RN 56263-51-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

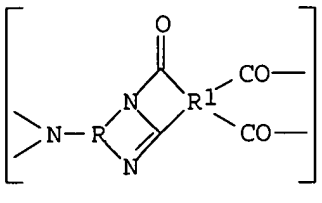


L3 ANSWER 157 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:165564 CAPLUS
DN 84:165564
TI Polymers prepared from aromatic diaminoalkoxycarboxylamine compounds and dianhydrides and method for their preparation
IN Miyadera, Yasuo; Yokokura, Hisao
PA Hitachi, Ltd., Japan
SO U.S., 14 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

10803578

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3926914	A	19751216	US 1973-413232	19731106
PRAI	US 1973-413232	A	19731106		

GI



n I

AB Reactions between aromatic diaminoalkoxycarbonylamino compds. and tetracarboxylic acid derivs. in inert solvents gave polyamic acid solns. which were storage-stable at room temperature for several months. These solns. were applied as protective-insulating coatings to metals or elec. cables and heated to evaporate the solvent and cyclyze the polyamic acids to heat-resistant polyimidazopyrrolones, such as I (R and R' are aromatic rings). Thus, 3,3'-diamino-4,4'-diethoxycarbonylaminodiphenyl ether-3,3',4,4'-benzophenonetetracarboxylic dianhydride polymer (II) [53189-56-3] obtained by stirring its monomers in N-methyl-2-pyrrolidone with cooling had reduced viscosity 1.33 dl/g, but in solution it did not gel for >6 months at room temperature Heating this solution in a shallow pan at 300-400° gave tough film which was stable at 470° in air and had semi-conductive properties. Analogously, 26 polymers similar to II were prepared

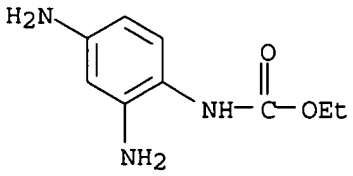
IT **58991-70-1**
RL: USES (Uses)
(storage-stable solns. of, for heat-resistant coatings)

RN 58991-70-1 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 2,4-bis(chlorocarbonyl)-, dimethyl ester, polymer with ethyl (2,4-diaminophenyl)carbamate (9CI) (CA INDEX NAME)

CM 1

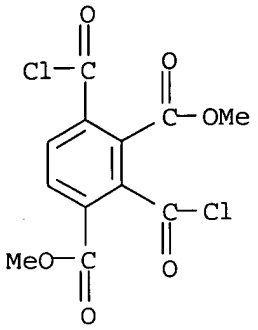
CRN 53189-44-9
CMF C9 H13 N3 O2



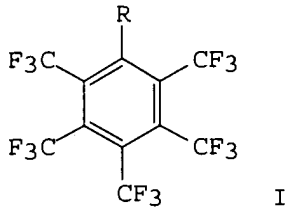
CM 2

CRN 19116-49-5
CMF C12 H8 Cl2 O6

10803578



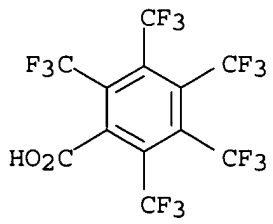
L3 ANSWER 158 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:150295 CAPLUS
DN 84:150295
TI Pentakis(trifluoromethyl)benzoic acid and pentakis(trifluoromethyl)aniline
AU Yagupol'skii, L. M.; Lukmanov, V. G.; Alekseeva, L. A.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1976), 12(2), 470
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI



I

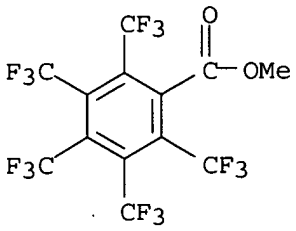
AB Reaction of C6(CF3)6 with NaOMe gave 92% I [R = C(OMe)3], which gave 95% I (R = CO2Me) (II) on treatment with concentrated H2SO4. Hydrolysis of II gave 64% I (R = CO2H), which was converted to 82% I (R = NH2) (III) on treatment with H2SO4 and NaN3. III reacted with p-Me2NC6H4CHO to give the resp. anil in 42% yield.

IT **58956-75-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to amine)
RN 58956-75-5 CAPLUS
CN Benzoic acid, pentakis(trifluoromethyl)- (9CI) (CA INDEX NAME)

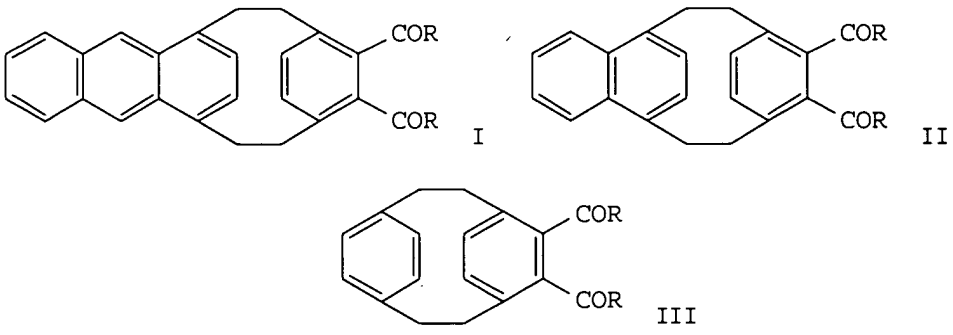


IT **6626-10-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and hydrolysis of)
RN 6626-10-4 CAPLUS
CN Benzoic acid, pentakis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

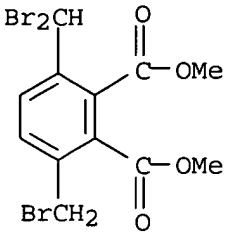


L3 ANSWER 159 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:134940 CAPLUS
DN 84:134940
TI Constitution and chemiluminescence, VII. Chemiluminescent paracyclophanes, II: Intramolecular sensitized chemiluminescence
AU Gundermann, Karl D.; Roeker, Klaus D.
CS Org.-Chem. Inst., Tech. Univ. Clausthal, Clausthal-Zellerfeld, Fed. Rep. Ger.
SO Justus Liebigs Annalen der Chemie (1976), (1), 140-52
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA German
OS CASREACT 84:134940
GI

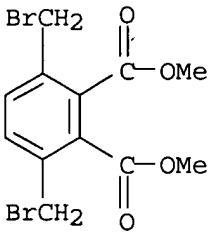


AB Reactions of paracyclophanes (I, II, III; R = MeO), prepared by ring contraction of the corresponding dithia[3.3]paracyclophanes, with absolute H2NNH2 gave cyclic hydrazides [I, II, and III (RR) = NHNH], which are chemiluminescent under oxidative conditions. In aprotic media, the intramol. sensitized chemiluminescence of I [(RR) = NHNH] reaches the quantum yield of luminol.
IT **58791-51-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58791-51-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-6-(dibromomethyl)-, dimethyl

ester (9CI) (CA INDEX NAME)



IT **43183-80-8**
RL: PRP (Properties)
(reaction with bis(mercaptomethyl) compds., dithia[3.3]paracyclophanes from)
RN 43183-80-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



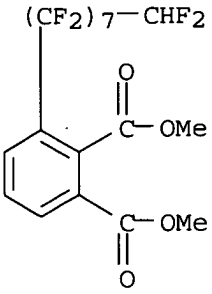
L3 ANSWER 160 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:89791 CAPLUS
DN 84:89791
TI Manufacture of fluoroalkyl aromatic compounds
IN Thrower, John
PA United Kingdom Secretary for Defence, UK
SO Brit., 4 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1416181	A	19751203	GB 1972-2100	19730117
PRAI	GB 1972-2100	A	19730117		

AB Three title compds. 2,3-R2C6H3(CF2)nCHF2 (R= H, n = 5, 7; R = CO2Me, n = 7) were prepared (5-60%) from Cl(CF2)nCHF2 by treatment in Me2SO with PhI or 3,2-Br(MeO2C)C6H3CO2Me, Cu bronze, and 2,2'-bipyridyl or 8-quinolinol for 2-5 hr at 120-40° under N. Ph(CF2)3Ph was prepared similarly (50%) from Cl(CF2)3Cl and PhI.

IT **58749-36-3P**
RL: PREP (Preparation)
(from di-Me bromophthalate)
RN 58749-36-3 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-hexadecafluorooctyl)-, dimethyl ester (9CI) (CA INDEX NAME)

10803578

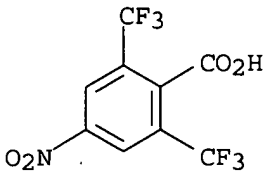


L3 ANSWER 161 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:31139 CAPLUS
DN 84:31139
TI 2-Phenyl-as-triazine-3,5(2H,4H)diones
IN Miller, Max W.
PA Pfizer Inc., USA
SO U.S., 17 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 5

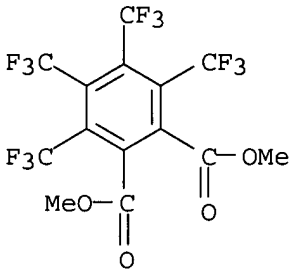
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3912723	A	19751014	US 1973-381062	19730720
	US 3560497	A	19710202	US 1968-768191	19681016
	GB 1371907	A	19741030	GB 1971-41743	19710907
	ZA 7106613	A	19720628	ZA 1971-6613	19711004
	IN 133131	A	19750823	IN 1971-133131	19711006
	FR 2110283	A5	19720602	FR 1971-36162	19711007
	FR 2110283	B1	19751031		
	AU 7134347	A1	19730412	AU 1971-34347	19711007
	AT 7108669	A	19750115	AT 1971-8669	19711007
	AT 325629	B	19751027		
	PL 88946	P	19761030	PL 1971-151572	19711113
PRAI	US 1968-768191	A2	19681016		
	US 1970-78917	A2	19701007		
	US 1971-129139	A2	19710329		
	GB 1971-41743	A	19710907		

GI For diagram(s), see printed CA Issue.
AB Phenyltriazinediones I(R = H, halo, CN; R1 = H, halo SMe, CF3, Me, NO2, OMe; R2 = H, halo, SO2Me, OMe, CN, Me substituted phenoxy, and phenylthio, H2NSO2 and N-substituted H2NSO2; R3 = H, Me, CF3, halo, NO2, OMe; R4 = H) (138 compds.), useful in the control of coccidiosis, were prepared Thus I(R = R3 = H, R1 = R2 = Cl, R4 = CO2H), obtained by coupling diazotized 3,4-Cl2C6H3NH2 with NCCH2CONHCO2Et followed by refluxing in 1N KOH, was decarboxylated to give I(R = R3 = R4 = H, R1 = R2 = Cl) which had a min. effective concentration of 0.006% in the control of Eimeria tenella in chicks.
IT **57715-98-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation chlorination of)
RN 57715-98-7 CAPLUS
CN Benzoic acid, 4-nitro-2,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 162 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:563679 CAPLUS
DN 83:163679
TI Perfluorotetramethylcyclopentadienone as a Diels-Alder diene
AU Szilagyi, S.; Ross, J. A.; Lemal, D. M.
CS Dep. Chem., Dartmouth Coll., Hanover, NH, USA
SO Journal of the American Chemical Society (1975), 97(19), 5586-8
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB Though stable as a monomer, perfluorotetramethylcyclopentadienone (I) is a highly reactive compound whose capabilities as a Diels-Alder addend are described. Reactions with olefins, acetylenes, dienes, and (cursorily) aromatic are explored. I is among the most powerful diene components in the Diels-Alder reaction with inverse electron demand, and it adds readily to electron-deficient dienophiles as well. Its high thermal and photochem. stability enhances its versatility as a trapping reagent. In its reaction with dienes, the dienone assumes the role of the diene component. The origin of its remarkable reactivity is discussed.
IT **57473-75-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57473-75-3 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrakis(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 163 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:497339 CAPLUS
DN 83:97339
TI 1-Phthalazone derivatives
IN Inoue, Michiro; Ishikawa, Masayuki; Tsuchiya, Takashi; Shimamoto, Takio
PA Japan
SO Ger. Offen., 35 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3
PATENT NO. KIND DATE APPLICATION NO. DATE

PI	DE 2451417	A1	19750507	DE 1974-2451417	19741029
	DE 2451417	B2	19800514		
	DE 2451417	C3	19810129		
	JP 50070378	A2	19750611	JP 1973-121260	19731030
	JP 57032065	B4	19820708		
	JP 50070380	A2	19750611	JP 1973-121757	19731031
	JP 57024786	B4	19820526		
	AU 7472954	A1	19760311	AU 1974-72954	19740904
	GB 1459606	A	19761222	GB 1974-38708	19740904
	US 3963716	A	19760615	US 1974-504745	19740910
	BE 819785	A1	19750311	BE 1974-148408	19740911
	IL 45675	A1	19781031	IL 1974-45675	19740916
	ZA 7406094	A	19751126	ZA 1974-6094	19740925
	FR 2248841	A1	19750523	FR 1974-35550	19741023
	SE 7413530	A	19750502	SE 1974-13530	19741028
	SE 412389	C	19800619		
	SE 412389	B	19800303		
	DK 7405618	A	19750707	DK 1974-5618	19741028
	DK 134345	B	19761025		
	FI 7403157	A	19750501	FI 1974-3157	19741029
	FI 59402	B	19810430		
	FI 59402	C	19810810		
	HU 168797	P	19760728	HU 1974-IO218	19741029
	ES 431454	A1	19761016	ES 1974-431454	19741029
	NL 7414186	A	19750502	NL 1974-14186	19741030
	DD 119231	C	19760412	DD 1974-182046	19741030
	AT 7408745	A	19761015	AT 1974-8745	19741030
	AT 337195	B	19770610		
	PL 100122	P	19780930	PL 1974-175246	19741030
	CH 610892	A	19790515	CH 1974-14546	19741030
	CH 611282	A	19790531	CH 1978-4978	19741030
	CS 194213	P	19791130	CS 1974-7404	19741030
	CS 194248	P	19791130	CS 1977-5416	19741030
	PL 117861	B1	19810831	PL 1974-201602	19741030
	ES 437041	A1	19770116	ES 1975-437041	19750426
	SU 563913	D	19770630	SU 1975-2199204	19751217
	IN 139552	A	19760703	IN 1976-CA330	19760225
	AT 7604711	A	19761115	AT 1976-4711	19760628
	AT 337709	B	19770711		
PRAI	JP 1973-121260	A	19731030		
	JP 1973-121757	A	19731031		
	AT 1974-8745	A	19741030		

OS CASREACT 83:97339

GI For diagram(s), see printed CA Issue.

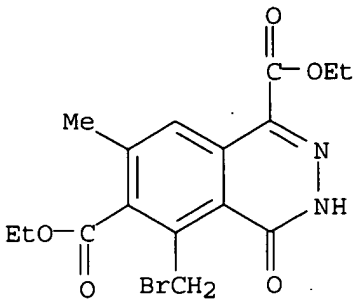
AB Phthalazone (I, R = CO2Et, R1 = CO2H) was obtained by treatment of phthalide (II) with KOH followed by reaction with N2H4.H2O. Subsequent esterification with EtOH-H2SO4 gave 90-5% I(R = R1 = CO2Et). Analogously obtained were I (R = CO2Me, R1 = CO2H, CO2Me). Reduction of the diester gave hydroxy ester (I, R = CO2Et, R1 = CH2Et,R1 = CH2OH). Bromination of I(R = R1 = CO2Et) with N-bromosuccinimide gave a bromomethyl derivative which was cyclized by heating at 185-90° to give III. The compds. were useful hypotensive agents and inhibited induced arteriosclerosis in rats.

IT **56611-74-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 56611-74-6 CAPLUS

CN 1,6-Phthalazinedicarboxylic acid, 5-(bromomethyl)-3,4-dihydro-7-methyl-4-oxo-, diethyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 164 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:497063 CAPLUS
DN 83:97063
TI 6,11-Dihydrodibenzo[b,e]-oxepinacetic acids and their derivatives
IN Helsley, Grover C.; McFadden, Arthur R.; Hoffman, David
PA Hoechst A.-G., Fed. Rep. Ger.
SO Ger. Offen., 31 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2442060	A1	19750507	DE 1974-2442060	19740903
	US 4585788	A	19860429	US 1974-459774	19740410
	NL 7411565	A	19750310	NL 1974-11565	19740830
	ES 429701	A1	19770216	ES 1974-429701	19740831
	CH 609960	A	19790330	CH 1978-6753	19740903
	CH 615172	A	19800115	CH 1974-11955	19740903
	FI 7402583	A	19750307	FI 1974-2583	19740904
	FI 66368	B	19840629		
	FI 66368	C	19841010		
	SE 7411156	A	19750307	SE 1974-11156	19740904
	AU 7472962	A1	19760415	AU 1974-72962	19740904
	AU 499709	B2	19790503		
	HU 172797	P	19781228	HU 1974-HO1716	19740904
	NO 7403203	A	19750307	NO 1974-3203	19740905
	NO 142397	B	19800505		
	NO 142397	C	19800813		
	DK 7404705	A	19750505	DK 1974-4705	19740905
	AT 7407164	A	19770715	AT 1974-7164	19740905
	CA 1153384	A1	19830906	CA 1974-208542	19740905
	BE 819637	A1	19750306	BE 1974-148288	19740906
	FR 2242976	A1	19750404	FR 1974-30329	19740906
	JP 50058084	A2	19750520	JP 1974-102876	19740906
	GB 1481866	A	19770803	GB 1974-39112	19740906
	ZA 7405665	A	19760225	ZA 1974-5665	19750905
	AT 7705637	A	19800115	AT 1977-5637	19770729
	AT 358014	B	19800811		
	US 4816591	A	19890328	US 1979-91159	19791105
PRAI	US 1973-394801	A	19730906		
	US 1974-459774	A	19740410		
	AT 1974-7164	A	19740905		

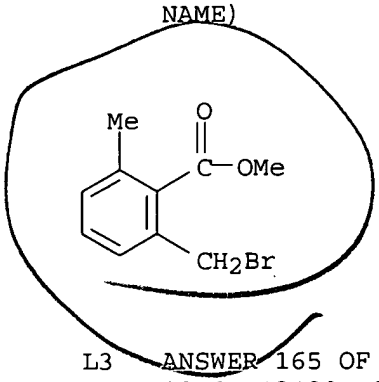
OS CASREACT 83:97063
GI For diagram(s), see printed CA Issue.
AB Dibenzoxepinacetic acids I (R = H, Me, CHMe2; R1R2 = O; R1 = H, R2 = OH, OMe; R3 = H, 7-Cl, 8-Cl, 9-Cl, 9-CF3, 8-OMe, 9-F, 10-Me) and some related compds. were prepared Thus 2-MeC6H4CO2Et was brominated and condensed with

4-HOC6H4CH2CO2H to give 4-(2-EtO2CC6H4CH2O)C6H4CH2CO2Et, which was hydrolyzed and cyclized to I (R = R3 = H, R1R2 = O, II). II had a ED50 in the carrageenin edema tests in rats of 6.5 mg/kg and an analgesic ED50 in the writhing test in mice of 7.6 mg/kg.

IT **56427-77-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with hydroxyphenylacetate)

RN 56427-77-1 CAPLUS

CN Benzoic acid, 2-(bromomethyl)-6-methyl-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 165 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1975:442490 CAPLUS

DN 83:42490

TI Steric interactions of inner atoms in cyclic compounds. XXII. Nitro, carboxy, sulfnyl, mercaptomethyl, and phenyl groups as intraanular substituents

AU Voegtle, Fritz; Gruetze, Joachim; Naetscher, Richard; Wieder, Wolfgang; Weber, Edwin; Gruen, Ralph

CS Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, Fed. Rep. Ger.

SO Chemische Berichte (1975), 108(5), 1694-711
CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 83:42490

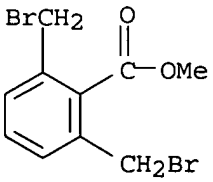
GI For diagram(s), see printed CA Issue.

AB The conformational inversion barriers (ΔG*) in I (R = NO2, CO2Me, MeS, MeSO2; n = 8, 10, 12) were determined by monitoring benzylic proton NMR absorptions at several temps. [R, n, ΔG* (kcal/mole) given: NO2, 8, 15.2; MeCO2, 10, 23.6; MeS, 10, 17.4; MeSO2, 12, 16.9]. Th NMR of other I were also examined

IT **56263-51-5P 56263-52-6P 56263-53-7P**
56288-24-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with alkanedithiol)

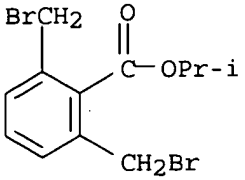
RN 56263-51-5 CAPLUS

CN Benzoic acid, 2,6-bis(bromomethyl)-, methyl ester (9CI) (CA INDEX NAME)

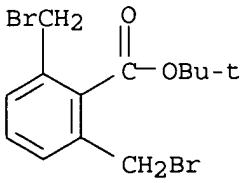


RN 56263-52-6 CAPLUS

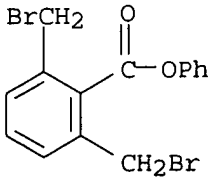
CN Benzoic acid, 2,6-bis(bromomethyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



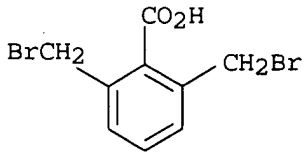
RN 56263-53-7 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 56288-24-5 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)-, phenyl ester (9CI) (CA INDEX NAME)



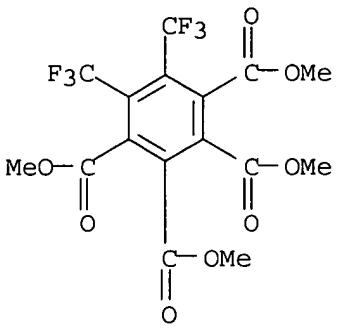
IT **56263-54-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 56263-54-8 CAPLUS
CN Benzoic acid, 2,6-bis(bromomethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 166 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:156482 CAPLUS
DN 82:156482
TI Acetylenes and noble metal compounds. XII. Reactions of dimethyl acetylenedicarboxylate with palladium(II) chloride and the structure of [[chloro(methoxycarbonyl)[1,2,3,4,5-pentakis(methoxycarbonyl)cyclopenta-2,4-dienyl]-2-MeOCO]methyl](pentane-2,4-dionato)palladium(II)
AU Roe, David; Calvo, Crispin; Krishnamachari, Narasimhan; Maitlis, Peter M.
CS Chem. Dep., McMaster Univ., Hamilton, ON, Can.
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1975), (2), 125-32

10803578

CODEN: JCDTBI; ISSN: 0300-9246
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB PdCl2 with MeO2CC.tplbond.CCO2Me gave [LPd(μ-Cl)2PdL] (I). The structure I was assigned spectroscopically and by x-ray anal. of [PdLL1] [L1H = (MeCO)2CH2] (II). Crystals of II.0.66CHCl3 were monoclinic, space group P2 1/c, with a 8.78, b 21.15, c 16.76 Å, β 93.0°, d.(observed) 1.55, and d.(calculated) 1.594 for Z = 4. The structure was refined to R 0.071 for 2396 reflections. Thermal or aqueous CN- decomposition of I gave C6(CO2Me)6. Analogs. of I and II were prepared by reaction of the σ-buta-1,3-dienyl complex [Pd[C4(CO2Me)4Br]Br]n with RC.tplbond.CR (R = CO2Me, CF3). The (CF3)2C2 product with aqueous CN- gave 5,6-(F3C)2C6(CO2Me)4. Degradation products of I were reformulated as the cyclopentadienes III (R = H, Cl, Br).
IT **52649-59-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52649-59-9 CAPLUS
CN 1,2,3,4-Benzenetetracarboxylic acid, 5,6-bis(trifluoromethyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

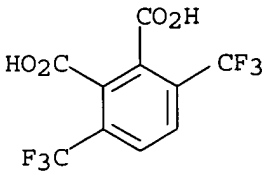


L3 ANSWER 167 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:551908 CAPLUS
DN 81:151908
TI Fluorination of aromatic carboxylic acids by sulfur tetrafluoride. XI. Fluorination of naphthalenecarboxylic acids
AU Kunshenko, B. V.; Alekseeva, L. A.; Yagupol'skii, L. M.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1974), 10(8), 1698-704
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Fluorination of 1,4,8-naphthalenetricarboxylic acid by SF4 at 220° gave 70% naphthopyran (I; R = R2 = R3 = H, R1 = CF3) which was hydrolyzed by H2SO4 to give 98% 4-trifluoromethyl-1,8-naphthalenedicarboxylic acid. Fluorination of 1,4,5,8-naphthalenetetracarboxylic acid with SF4 in the presence of HF at 240° gave 80% naphthodipyran (II). Fluorination of4-nitro-1,8-napthalenedicarboxylic acid with SF4 at 150° gave 98% naphthopyran (III) which was fluorinated at 250° to yield 85% I (R = R2 = R3 = H, R1 = NO2). 3,6-Dintro-1,8-naphthalenedicarboxylic acid fluorinated with SF4-HF gave quant.I (R = R3 = NO2, R1 = R2 = H). Analogously the 4,5-dinitro acid gave 80% I (R = R3 = H, R1 = R2 = NO2).

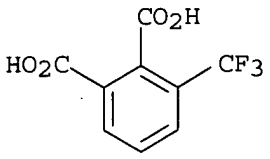
acenaphthene IV was obtained in 99% yield by fluorination of the corresponding acenaphthenequinone with SF4-HF at 150°.

IT **24866-16-8P 24913-62-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24866-16-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



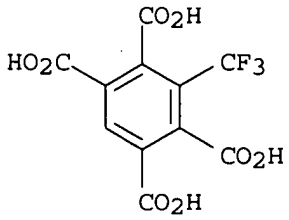
RN 24913-62-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 168 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:551664 CAPLUS
DN 81:151664
TI Penta(trifluoromethyl)benzene
AU Lukmanov, V. G.; Alekseeva, L. A.; Yagupol'skii, L. M.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1974), 10(9), 2000-1
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Treatment of the iodobenzene I (R = iodo) with CF3I and Cu gave 65% I (R = CF3), which was oxidized with HNO3 to give 89% the carboxylic acid II (R1 = CO2H); the latter gave 53%II (R1 = CF3) with SF4-HF.

IT **53812-59-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorination of)

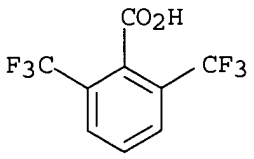
RN 53812-59-2 CAPLUS
CN 1,2,4,5-Benzenetetracarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 169 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:491232 CAPLUS
DN 81:91232
TI Bis(trifluoromethyl)benzamides
IN Houlihan, William J.
PA Sandoz-Wander, Inc.
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3825594	A	19740723	US 1971-156459	19710624
PRAI	US 1970-4397	A2	19700120		

GI For diagram(s), see printed CA Issue.
AB Six benz-amides [I; R = H, Me2N(CH2)3, cyclohexyl, CH.tplbond.CCMe2; x = 4,5], with central nervous system depressant activity in mice and coccidiostatic activity in poultry, were prepared from 1,4- (II) or 1,3-(F3C)2C6H4 (III) by a series of reactions. Thus, II and III were carboxylated via their Li derivs. II gave 2,5-, and III gave a mixture of 2,4- and 2,6- (F3C)2C6H3CO2H in which 2,4-acid predominated. The mixture was separated via gas chromatog. of Me esters. The benzoic acids were converted to their acid chlorides which were treated with RNH2 to give I.
IT **24821-22-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with thionyl chloride)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 170 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:133597 CAPLUS
DN 80:133597
TI Alkenyl complexes of iridium and their properties as cyclotrimerization catalysts
AU Baddley, William H.; Tupper, G. B.j
CS Coates Chem. Lab., Louisiana State Univ., Baton Rouge, LA, USA
SO Journal of Organometallic Chemistry (1974), 67(1), C16-C18
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
AB Reactions of activated, disubstituted acetylenes with IrH(CO)(PPh3)3 under various conditions give 4-, 5-, and 6-coordinate alkenyliridium complexes. Some new, novel alkenyl metallocycles containing 2 different acetylenic units incorporated into the metallocyclopentadiene ring were also prepared, and these are good catalysts for the cyclotrimerization of disubstituted acetylenes.
IT **52649-59-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

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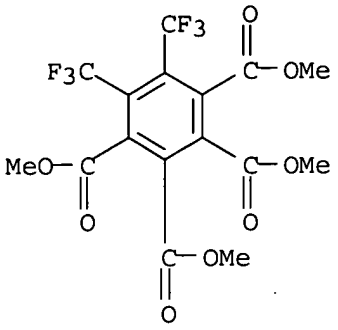
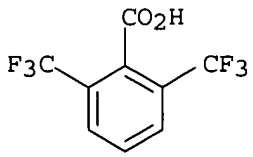
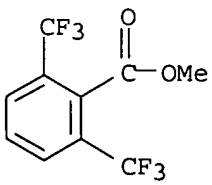
RN 52649-59-9 CAPLUS
CN 1,2,3,4-Benzenetetracarboxylic acid, 5,6-bis(trifluoromethyl)-, tetramethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 171 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:133521 CAPLUS
DN 80:133521
TI Metalation of 1,3-bis(trifluoromethyl)benzene by butyllithium
AU Aeberli, Paul; Houlihan, William J.
CS Res. Dev. Div., Sandoz-Wander Inc., Hanover, NJ, USA
SO Journal of Organometallic Chemistry (1974), 67(3), 321-5
CODEN: JORCAI; ISSN: 0022-328X
DT Journal
LA English
AB Treatment of the Li reagent from 1,3-bis(trifluoromethyl)benzene (I) with CO2 gave a 60-40 mixture of 2,4- and 2,6-bis(trifluoromethyl) benzoic acids. The lithiation-carbonation of 1,3-bis(trifluoromethyl)benzene-5-d gave the same acids without loss of deuterium. This result indicates that I, unlike trifluoromethylbenzene, does not lithiate meta to a CF3 group.
IT **24821-22-5P 34060-79-2P 52148-51-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

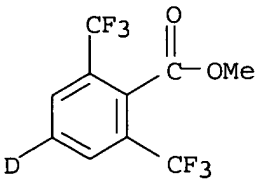


RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)

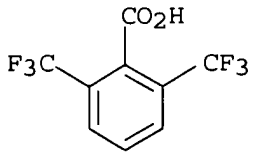


10803578

RN 52148-51-3 CAPLUS
CN Benzoic-4-d acid, 2,6-bis(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

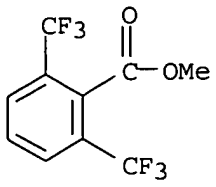


L3 ANSWER 172 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:55272 CAPLUS
DN 80:55272
TI Electroorganic reactions. I. Cathodic cleavage in methanol solution of benzylic carbon-oxygen and carbon-fluorine bonds
AU Coleman, James P.; Naser-ud-din; Gilde, Hans D.; Utley, James H. P.; Weedon, Basil C. L.; Eberson, Lennart
CS Dep. Chem., Queen Mary Coll., London, UK
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1973), (14), 1903-8
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
AB Controlled potential electroredn. of MeOH solns. of p-MeOρCC6H4CH2OR (R = Ac, Me) gave 71-95% p-MeO2CC6H4Me with a current efficiency of 50-76%. Similarly, substituted benzotrifluorides were cleaved to the appropriate substituted toluenes. Efficient reduction required electron-accepting substituents, CO2Me or CN, para to the group undergoing cleavage. The effect of substituents and AcOH on the product distribution, together with voltammetric data, indicated an e.c.e. mechanism.
IT **24821-22-5P**
RL: PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

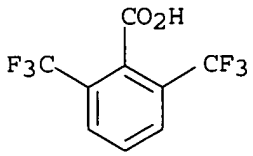


IT **34060-79-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, polarog., in methanol)
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)

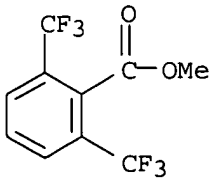
10803578



L3 ANSWER 173 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:36404 CAPLUS
DN 80:36404
TI NMR study of substituted 1,3- and 1,4-bis(trifluoromethyl)benzenes
AU Bartle, K. D.; Hallas, G.; Hepworth, J. D.
CS Dep. Colour Chem., Univ. Leeds, Leeds, UK
SO Organic Magnetic Resonance (1973), 5(10), 479-81
CODEN: ORMRBD; ISSN: 0030-4921
DT Journal
LA English
AB Metalation of 1,3-bis(tri-fluoromethyl)benzene with BuLi occurred at the 2- and 4-positions. Lithiation of 1,4-bis(trifluoromethyl)benzene and subsequent carboxylation gave the 2-carboxylic acid. Structures were assigned using 100 and 220 MHz PMR data. Coupling effects between aromatic protons and CF3 groups and the aromatic chemical shifts induced by esterification were examined for bis(tri-fluoromethyl)benzoic acids.
IT **24821-22-5 34060-79-2**
RL: PRP (Properties)
(NMR of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



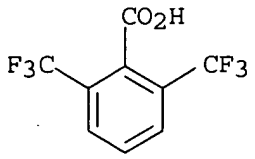
L3 ANSWER 174 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1973:491787 CAPLUS
DN 79:91787
TI Bis(trifluoromethyl)benzoic acids
IN Houlihan, William J.
PA Sandoz-Wander, Inc.
SO U.S., 3 pp.
CODEN: USXXAM

10803578

DT Patent
LA English
FAN.CNT 1

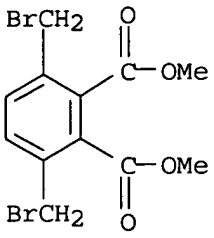
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3751491	A	19730807	US 1970-27459	19700410
PRAI	US 1968-703880	A2	19680208		

GI For diagram(s), see printed CA Issue.
AB The title benzoic acids (I, F3C position 4-, 5-, 6-), useful as herbicides and central nervous system depressants, were prepared by lithiating 1,4- and 1,3-C6H4(CF3)2 (II) with LiBu and treating the products with CO2. II gave a mixture of 2,4- and 2,6-acids in which the 2,4-isomer predominated.
IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

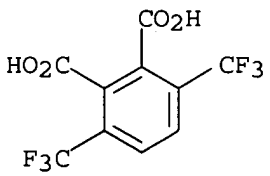


L3 ANSWER 175 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1973:478766 CAPLUS
DN 79:78766
TI Constitution and chemiluminescence. 5. Chemiluminescent paracyclophanes
AU Gundermann, Karl D.; Roeker, Klaus D.
CS Org.-Chem. Inst., Tech. Univ. Clausthal, Clausthal-Zellerfeld, Fed. Rep. Ger.
SO Angewandte Chemie (1973), 85(10), 451-2
CODEN: ANCEAD; ISSN: 0044-8249
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB Reaction of the phthalate 3,6-(BrCH2)2C6H2(CO2Me)2-1,2(I) with p-(NaSCH2)2C6H4 gave 30% dithia compound II, which on oxidation gave 65% disulfone (III). Pyrolysis of III in the presence of terphenyl gave 25% paracyclophane IV (R = R1 = OMe), which on reaction with N2H4.H2O gave the paracyclophane IV (RR1 = NHNH) (V). Reaction of I with VI and NaOH gave 31% dithia compound VII (R = R1 = OMe), which on reaction with N2H4 gave the paracyclophane VII (R = R1 = NHNH) (VIII). The paracyclophanes V and VIII showed chemiluminescence on oxidation with O/BuOK/Me2SO.
IT **43183-80-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with arylenebis(methanethiol) derivs.)
RN 43183-80-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

10803578

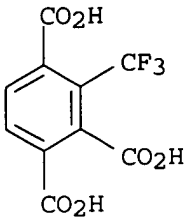


L3 ANSWER 176 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1973:418610 CAPLUS
DN 79:18610
TI Fluorination of aromatic carboxylic acids by sulfur tetrafluoride. VIII. Fluorination of spatially hindered aromatic carboxylic acids
AU Yagupol'skii, L. M.; Burmakov, A. I.; Alekseeva, L. A.; Kunshenko, B. V.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1973), 9(4), 689-96
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Fluorination of benzenetricarboxylic acid (I; R = R1 = R2 = CO2H) by SF4 gave 76% fluoride (I; R = R2 = CF3, R1 = COF) which was hydrolyzed to yield 73% acid (I; R = R2 = CF3, R1 = CO2H). The latter was decarboxylated by heat to give 67% (I; R = R2 = CF3, R1 = H). Analogous fluorination of benzenetetracarboxylic acid (II) gave 84% benzodifuran (III; R = Br). Naphthopyran (IV) was obtained in 63% yield from naphthalic acid. Treatment of mellitic acid by SF4 gave 65% III (R = CF3) and 55% benzotrifuran (V) was obtained by fluorination of the corresponding perchlorobenzotrifuran.
IT **24866-16-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of, by sulfur tetrafluoride)
RN 24866-16-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

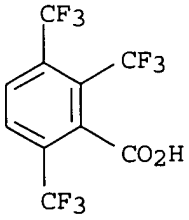


IT **41819-00-5P 41819-04-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41819-00-5 CAPLUS
CN 1,2,4-Benzenetricarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

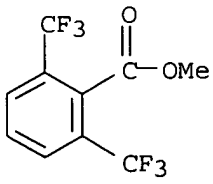
10803578



RN 41819-04-9 CAPLUS
CN Benzoic acid, 2,3,6-tris(trifluoromethyl)- (9CI) (CA INDEX NAME)

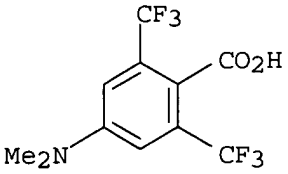


L3 ANSWER 177 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1973:29040 CAPLUS
DN 78:29040
TI Dipole moment study of the ortho-effects of methyl and trifluoromethyl groups
AU Hepworth, J. D.; Ibbitson, D. A.; Williams, A. J.; Hallas, G.
CS Dep. Chem. Mater. Sci., Derby Coll. Art Technol., Derby, UK
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1972), (15), 2298-9
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
AB Apparent dipole moments in C6H6 of the Me esters of 2-methyl-, 2,6-dimethyl-, 2-(trifluoromethyl)-, and 2,6-bis(trifluoromethyl)benzoic acid (I) were determined The moments of the 2-substituted esters were explained by disturbance of the conjugation between the ester and Ph groups by the electronic effects of the ortho-groups and by a twisting of the ester group out of the plane of the benzene ring. The moments of the 2,6-disubstituted esters were independent of the angular displacement of the ester group and the important contribution of lone-pair repulsions between the substituents in I to the dipole moment was established.
IT **34060-79-2**
RL: PRP (Properties)
(dipole moment of)
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)

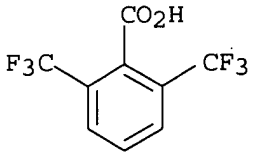


10803578

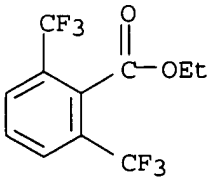
L3 ANSWER 178 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1972:539544 CAPLUS
DN 77:139544
TI Esterification of 2,6-bis(trifluoromethyl)benzoic acid
AU Hallas, G.; Hepworth, J. D.
CS Dep. Colour Chem., Univ. Leeds, Leeds, UK
SO Chemistry & Industry (London, United Kingdom) (1972), (17), 691-2
CODEN: CHINAG; ISSN: 0009-3068
DT Journal
LA English
AB 2,6-(F3C)2C6H3CO2R (I, R = H) reacted with Me2SO4 and Et2SO4 in aqueous alkali-dioxane to give .apprx.90% I (R = Me and Et, resp.). 4,2,6-(Me2N)(F3C)2C6H2CO2H and 2,6-(O2N)2C6H3-CO2H reacted similarly with Me2SO4 to give the corresponding Me esters.
IT **34060-82-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, by dimethyl sulfate)
RN 34060-82-7 CAPLUS
CN Benzoic acid, 4-(dimethylamino)-2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



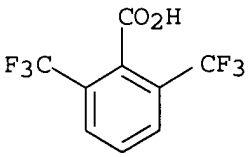
IT **24821-22-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of,by dimethyl and diethyl sulfates)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



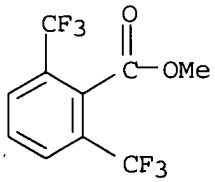
IT **38570-08-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38570-08-0 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)



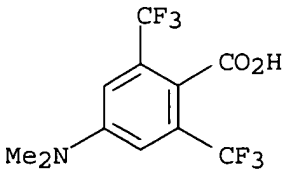
L3 ANSWER 179 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:540393 CAPLUS
DN 75:140393
TI Metalation of 1,3-bis(trifluoromethyl)benzene and N,N-dimethyl-3,5-bis(trifluoromethyl)aniline
AU Hepworth, J. D.; Grocock, D. E.; Jones, T. K.; Hallas, G.
CS Chem. Dep., Coll. Technol., Derby, UK
SO Journal of the Chemical Society [Section] C: Organic (1971), (19), 3305-8
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
OS CASREACT 75:140393
AB Metalation of m-(CF3)2C6H4 with BuLi-Me2N(CH2)2NMe2 occurs at the 2 position but with BuLi gives a mixture of products. 3,5-(CF3)2C6H3NMe2 reacts with BuLi at the 4 position and with Br2-H2O to give a 2,6(or 4)-di-Br derivative
IT **24821-22-5P 34060-79-2P 34060-82-7P 34060-83-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



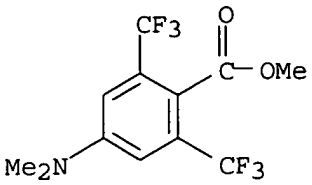
RN 34060-79-2 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



RN 34060-82-7 CAPLUS
CN Benzoic acid, 4-(dimethylamino)-2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



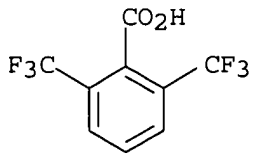
RN 34060-83-8 CAPLUS
CN Benzoic acid, 4-(dimethylamino)-2,6-bis(trifluoromethyl)-, methyl ester (8CI) (CA INDEX NAME)



L3 ANSWER 180 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:463428 CAPLUS
DN 75:63428
TI Substituted halobenzoic acids as plant growth regulators
IN Houlihan, William J.
PA Sandoz Ltd.
SO Ger. Offen., 19 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2060063	A	19710616	DE 1970-2060063	19701207
	US 3709938	A	19730109	US 1969-884011	19691210
	NL 7017936	A	19710614	NL 1970-17936	19701209
	FR 2073160	A5	19710924	FR 1970-44314	19701209
	ZA 7008319	A	19720726	ZA 1970-8319	19701209
PRAI	US 1969-884011	A	19691210		

GI For diagram(s), see printed CA Issue.
AB The title compds. (I), useful as plant growth regulators, were prepared by reaction of the phenyllithium compds. with CO2. Thus, a 15% solution of BuLi in hexane was added to 2,4-F2C6H3Me in THF at -15° and the mixture poured onto CO2-Et2O to give I (R = R3 = F, R1 = Me, R2 = H). Similarly prepared were I (R, R1, R2, and R3 given): CF3, H, H, CF3; CF3, H, CF3, H; Cl, Me, H, F; F, Me, H, Cl; Cl, Cl, H, F; F, F, F, F; Cl, MeO, H, Cl; F, H, H, CF3; Cl, CH2.CHCH2O, H, Cl; Cl,H, H, CF3.
IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 181 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:449615 CAPLUS
DN 75:49615
TI Synthesis of polyimides by the two-stage polycyclization of 2,5-diaromaticmethoxycarbonylterephthaloyl chloride with diamines
AU Korshak, V. V.; Vinogradova, S. V.; Vygodskii, Ya. S.; Gerashchenko, Z. v.
CS Inst. Elementoorg. Soedin., Moscow, USSR
SO Vysokomolekulyarnye Soedineniya, Seriya A (1971), 13(5), 1190-8

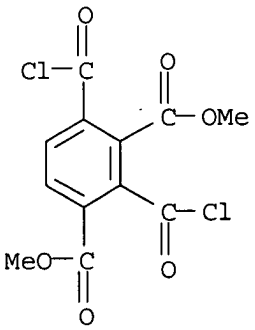
CODEN: VYSAAF; ISSN: 0507-5475
DT Journal
LA Russian

AB Polyamidoesters with hydrolytic stability were synthesized by polycondensation of 2,5-dicarbomethoxyterephthaloyl chloride with anilinephthalein, 9,9-bis(4-aminophenyl)-fluorene (anilinefluorene), 9,9-bis(4-aminophenyl)-10-anthrone (anilineanthrone), 4,4'-diaminodiphenyl ether, benzidine, and piperazine at 5-20° in MeCONMe2. Heating powdered 2,5-dicarbomethoxyterephthalic acid-anilinephthalein copolymer, 2,5-dicarbomethoxyterephthalic acid-anilinefluorene copolymer, and 2,5-dicarbomethoxyterephthalic acid-anilineanthrone copolymer at 200° for 3 hr in an inert atmospheric gave anilinephthalein polypyromellitimide, anilinefluorene polypyromellitimide, and anilineanthrone polypyromellitimide, resp.

IT **32824-04-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32824-04-7 CAPLUS
CN Isophthalic acid, 2,4-bis(chloroformyl)-, dimethyl ester, polyamide with benzidine and dimethyl 2,5-bis(chloroformyl)terephthalate (8CI) (CA INDEX NAME)

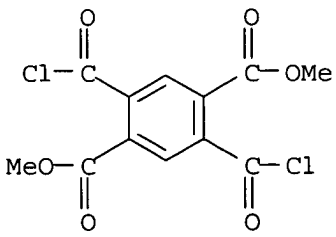
CM 1

CRN 19116-49-5
CMF C12 H8 Cl2 O6



CM 2

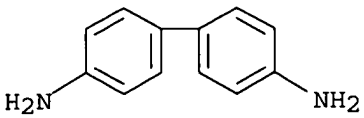
CRN 19014-14-3
CMF C12 H8 Cl2 O6



CM 3

10803578

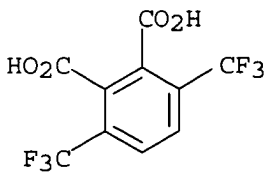
CRN 92-87-5
CMF C12 H12 N2



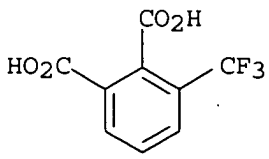
L3 ANSWER 182 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:99650 CAPLUS
DN 74:99650
TI O-Trifluoromethyl substituted phthalic acid
IN Burmakov, A. I.; Alekseeva, L. A.; Dashevskii, M. M.; Kotlov, A. N.; Shamis, E. M.; Yagupol'skii, L. M.
PA Institute of Organic Chemistry, Academy of Sciences, Ukrainian S.S.R.; Odessa Polytechnic Institute
SO U.S.S.R.
From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1970, 47(24), 24.
CODEN: URXXAF
DT Patent
LA Russian
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 276938		19700722	SU	19690626

AB o-Trifluoromethyl substituted phthalic acid was prepared from vicinal polycarboxylic acids, such as hemimellitic acid, by treating them with SF4 at 100-50°.
IT **24866-16-8P 24913-62-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24866-16-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



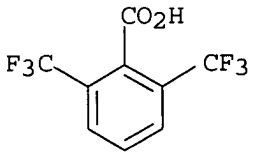
RN 24913-62-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 183 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN

10803578

AN 1970:446617 CAPLUS
DN 73:46617
TI Steric and electronic effects in basic dyes. I. Electronic absorption spectra of derivatives of malachite green containing trifluoromethyl groups in the phenyl ring
AU Hallas, Geoffrey; Grocock, D. E.; Hepworth, J. D.
CS Dep. Colour Chem. Dyeing, Univ. Leeds, Leeds, UK
SO Journal of the Society of Dyers and Colourists (1970), 86(5), 200-2
CODEN: JSDCAA; ISSN: 0037-9859
DT Journal
LA English
AB The electronic absorption spectra of malachite green derivs. containing CF3 groups in the phenyl ring were studied. Substituents in the 3-, 4-, or 3,5- positions had little effect on the maximum intensity of the first-frequency band, but they modified the position of the band to an extent linearly related to the appropriate Hammett substituent constant Although a substituent in the 2-position increased the intensity of the first band, the expected bathochromic shift relative to that of the 4-substituted isomer was not observed Steric hindrance of the central C atom in the 2-CF3 and 2,6-(CF3)2 derivs. facilitated nucleophilic replacement of a terminal Me2N group by a OH group with formation of a fuchsone. The hindrance was sufficient to permit replacement of a Me2N group in the corresponding dye bases.
IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

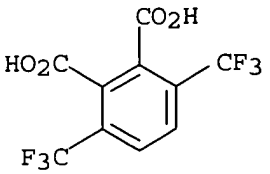


L3 ANSWER 184 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1970:89975 CAPLUS
DN 72:89975
TI Fluorination of aromatic polycarboxylic acids by sulfur tetrafluoride. III. Fluorination of benzenetetracarboxylic acids
AU Burmakov, A. I.; Alekseeva, L. A.; Yagupol'skii, L. M.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1970), 6(1), 144-8
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
AB Heating HO2CC6H2(CO2H)3-2,3,5 with SF4 in an autoclave ≤200° gave 2,4,6-(F3C)3C6H2COF (I). However, the fluorination of HO2CC6H2(CO2H)3-2,3,4 gave 4,7-bis(trifluoromethyl)-1,1,3,3-tetrafluorophthalan (II). The structure of I was proven by its stepwise conversion to 2,4,6-(F3C)2C6H2CONH2 (III), 2,4,6-(F3C)3C6H2NH2 (IV), 3,5-(F3C)2C6H3CF3, and HO2C-C6H3(CO2H)2-3,5. Heating III with P2O5 gave 2,4,6-(CF3)2-C6H2CN. The diazotization of IV followed by coupling with 3-MeC6H4N(CH2CH2OH)2 gave 2,4-Me[(HOCH2CH2)2N]-C6H3N:NC6H2(CF3)3-1,3,5. The structure of II was proved by its hydrolysis to 2,3,6-HO2C(F3C)2C6H2CO2H, which was converted to 4,7-bis(trifluoromethyl)phthalide (V). The treatment of V with PCl5 gave 4,7-bis(trifluoromethyl)-1,1,3,3-tetrachlorophthalan, which reacted with

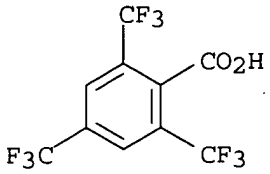
SbF3 to give II.

IT **24866-16-8P 25753-26-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24866-16-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 25753-26-8 CAPLUS
CN Benzoic acid, 2,4,6-tris(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 185 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1970:43737 CAPLUS
DN 72:43737
TI 1,2,8,9-Tetraazaphenalenes useful as cardiovascular agents
IN Doebel, Karl J.; Francis, John E.
PA Geigy Chemical Corp.
SO U.S., 4 pp. Continuation-in-part of U.S. 3429882
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

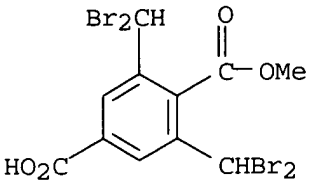
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3479355	A	19691118	US 1968-767819	19681015
PRAI US 1968-767819	A	19681015		

GI For diagram(s), see printed CA Issue.
AB Title compds. e.g. 1,2,8,9-tetraazaphenalene (I) are prepared by refluxing a 2,6-disubstituted benzoic acid derivative with hydrazine in aqueous mixture Two methods are used: 2,6-bis(dibromomethyl)benzoic acid (II) or the chloro derivative, is refluxed with two or molar equivalent NH2NH2 (III) in aqueous mixture until ring closure is complete; or a 2-carbonyl-6-formylbenzoic acid, or its tautomeric equivalent, i.e., 3-hydroxy-7-formylphthalide (IV), are treated in a similar fashion. Thus, 20 ml 100% III, 180 ml H2O, and 9.3 g II is refluxed 95 hr to give 2.17 g I, sublimes 190-240°, decomposed 294-8°. Also prepared were (m.p. given): II, 203-6°; IV, 127-33° (C6H6-hexane); 4-methoxy-2,6-bis(dibromomethyl)benzoic acid, 201-2° (C6H6) (90% yield); 3-hydroxy-5-methoxy-7-formylphthalide, 174-5° (C6H6) (36% yield); 5-methoxy - 1,2,8,9 - tetraazaphenalene, 291-4° (EtOH-EtOAc) (15.5% yield);

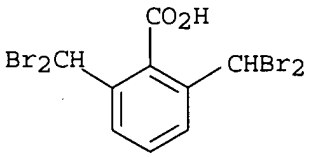
4-bromo-2,6-bis(dibromomethyl)benzoic acid, 220-1° (C6H6) (88% yield); 3-hydroxy-5-bromo-7-formyl-phthalide, 187-9°; 5-bromo-1,2,8,9-tetraazaphenalene, >35°; methyl4-carboxy-2,6-bis(dibromomethyl)benzoate, 211.5-13° (C6-H6-hexane); 5-carboxy-1,2,8,9-tetraazaphenalene, >34°; 3-hydroxy-3-phenyl-7-dibromomethylphthalide, 166-70° (C6H6-hexane); 3-hydroxy-7-benzoylphthalide, 109-11° (C6H6-hexane); 7-phenyl-1,2,8,9-tetraazaphenalene, 292-3° (EtOH); 4-butoxy-2,6-bis(dibromomethyl)benzoic acid, 187-8° (C6H6); 5-butoxy-1,2,8,9-tetraazaphenalene, 229-37°. Examples of both methods of preparation are given as well as those for preparation of intermediates.

IT **14346-63-5P 14346-75-9P 15562-75-1P 15562-76-2P 15562-77-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

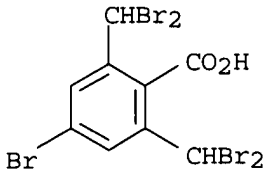
RN 14346-63-5 CAPLUS
CN Terephthalic acid, 2,6-bis(dibromomethyl)-, 1-methyl ester (8CI) (CA INDEX NAME)



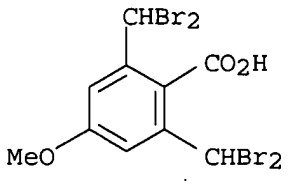
RN 14346-75-9 CAPLUS
CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 15562-75-1 CAPLUS
CN Benzoic acid, 4-bromo-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)

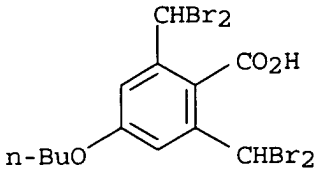


RN 15562-76-2 CAPLUS
CN p-Anisic acid, 2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)



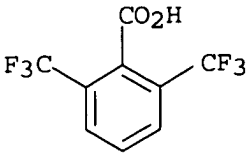
10803578

RN 15562-77-3 CAPLUS
CN Benzoic acid, 4-butoxy-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)

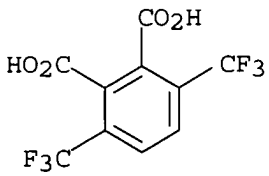


L3 ANSWER 186 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1970:31385 CAPLUS
DN 72:31385
TI Fluorination of aromatic polycarboxylic acids by sulfur tetrafluoride. I. Effect of spatial factors
AU Yagupol'skii, L. M.; Burmakov, A. I.; Alekseeva, L. A.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Obshchei Khimii (1969), 39(9), 2053-6
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
AB Heating 2.5 g hemimellitic acid and 14 g 80% SF4 in an autoclave 3 hr at 100-50°, then 5 hr at 160° and 7 hr at 175° gave 84% 2,6-bis(trifluoromethyl)benzoyl fluoride, b80 105-6°, n28D 1.3920, d28 1.5208, which with dry NH3 gave the amide, m. 198-9°. The fluoride and concentrated H2SO4 heated 2 hr at 60° gave the free acid, m. 136-7°, while the amide treated with KOBr in aqueous KOH at 0°, then 20 min at 75-85°, gave 67% 2,6-(F3C)2C6H3NH2, b20 60°, 1.4275, 1.4645; N-Ac derivative m. 175-7°. The amine (0.5 g) in 2.5 ml concentrated H2SO4 was added at 10° to 0.25 g NaNO2 in 2.5 ml concentrated H2SO4 and the mixture kept 1 hr, then quenched in ice, yielded a solution of the diazonium salt, which added to 3.5 g NaOP(O)H2 in 3.5 ml H2O and 3 ml concentrated H2SO4 gave in 10 hr at 20°, followed by steam distillation, 64% 1,3-C6H4(CF3)2, n30D 1.3761, which with concentrated H2SO4 and a trace of 30% oleum in 1.5 hr at 140-50° gave 77.5% isophthalic acid. Heating 3 g 3 nitrophthalic acid with 8.5 g 80% SF4 as above 2 hr at 100-20°, 3 hr at 130°, and 3 hr at 140°, gave on treatment of the crude product with NH3 84.5% 2-nitro-6-trifluoromethylbenzamide, m. 207-8°, and 7.1% more soluble 2,3-bis(trifluoromethyl)nitrobenzene, m. 26-8°, n25D 1.4360. The amide in aqueous H2SO4 treated with NaNO2 at 100° 20 min gave 72% 2-nitro-6-trifluoromethylbenzoic acid, m. 142-3°; the amide treated with KOBr in aqueous KOH, finally at 85°, gave 2-nitro-6-trifluoromethylaniline, m. 54°, which was hydrogenated over Pt in MeOH to 2,3-diaminobenzotrifluoride, m. 39-40°. 4-Nitrophthalic acid and SF4 as above at 100-40° gave 80% 3,4-(F3C)2C6H3NO2, b5 72°, n23D 1.4385. Thus, fluorination of hindered aromatic acids with SF4 is stereospecific and the reaction is affected by steric rather than electronic factors.
IT **24821-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24821-22-5 CAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)- (8CI, 9CI) (CA INDEX NAME)

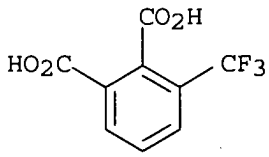
10803578



L3 ANSWER 187 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1970:21463 CAPLUS
DN 72:21463
TI Synthesis of o-trifluoromethyl derivatives of phthalic acids
AU Burmakov, A. I.; Alekseeva, L. A.; Yagupol'skii, L. M.
CS Inst. Org. Khim., Kiev, USSR
SO Zhurnal Organicheskoi Khimii (1969), 5(10), 1892-3
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB Heating hemimellitic acid with SF4 in an autoclave at 100° gave 3-(trifluoromethyl)phthalic difluoride which was converted by refluxing in 10% KOH solution to 3-(trifluoromethyl)phthalic acid (I). Heating I >170° gave I anhydride. Similarly, prehnitic acid was converted to 1,4-bis-(trifluoromethyl)phthalic acid and its anhydride.
IT **24866-16-8P 24913-62-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24866-16-8 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3,6-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 24913-62-0 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 188 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:512964 CAPLUS
DN 71:112964
TI 1,2,8,9-Tetraazaphenalenes
PA Geigy, J. R., A.-G.
SO Fr., 10 pp.
CODEN: FRXXAK
DT Patent
LA French

10803578

FAN.CNT 1 -

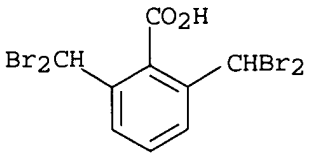
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1550404		19681220		
PRAI	US		19661030		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are sedatives and hypotensives. 2,6-Me2C6H3CO2H (36 g.) in 120 ml. CCl4 refluxed and treated in 30 min. with 75 g. Br in 350 ml. CCl4 under illumination with a 250-w. lamp, cooled, and filtered gave 2,6-(Br2CH)2C6-H3CO2H (II), m. 203-6°. II (9.3 g.), 180 ml. H2O, and 20 ml. N2H4.H2O (III) refluxed 95 hrs. gave 1,2,8,9-tetraazaphenalene (IV), m. 294-8° (decomposition). 3-Methylphthalic anhydride (81 g.), 182 g. N-bromosuccinimide (NBS), 40 mg. Bz2O2, and 1500 ml. CCl4 refluxed and irradiated with a 100-w. uv lamp, the mixture treated with 40 mg. more Bz2O2, stirred and refluxed 24 hrs. gave 72% 3-(dibromomethyl)phthalic anhydride (V), m. 93-5°. V (80 g.) in 500 ml. EtOH treated dropwise with a solution of 100 ml. III in 100 ml. H2O with stirring and cooling, and the mixture refluxed 88 hrs. and worked up gave 25.7 g. 3-hydroxy-1,2,8,9-tetraazaphenalene (VI), m. >350° (HCONMe2). V (40 g.) added slowly to 500 ml. 2N NaOH and the mixture acidified after 10 min. with HCl and heated 30 min. to 80° gave 7-carboxy-3-hydroxyphthalide (VII), m. 165.5-8.5° (H2O). VII (5.82 g.), 100 ml. AcOH and 3.6 ml. PhNHNH2 refluxed 18 hrs., and the mixture evaporated in vacuo gave 8-carboxy-2-phenyl-1(2H)-phthalazinone (VIII), m. 197-8° (C6H6). 3-Benzoylphthalic acid (32.5 g.), 145 ml. H2O, and 85 ml. III refluxed 18 hrs. gave 8-carboxy-4-phenyl-1 (2H)-phthalazinone, m. 257-9° (AcOH). VIII (24.3 g.), 40 ml. SOCl2, and 150 ml. PhCl refluxed 2 hrs., the mixture evaporated in vacuo, the residue dissolved in 350 ml. EtOH, and the solution refluxed 18 hrs. gave 8-ethoxycarbonyl-2-phenyl-1(2H)-phthalazinone (IX), m. 150-1°. Similarly was prepared 8-methoxycarbonyl-4-phenyl-1(2H)-phthalazinone, m. 198-202° (MeOH). IX (11.76 g.), 40 ml. 100% III, and 160 ml. Me Cellosolve refluxed 25 hrs. gave 3-oxo-9-phenyl-2,3-dihydro-1,2,8,9-tetraazaphenalene, m. 255-7° (Me Cellosolve). Similarly prepared was 3-oxo-7-phenyl-2,3-dihydro-1,2,8,9-tetraazaphenalene, m. >350°. 2-Benzoyl-6-methylbenzoic acid (2.4 g., m. 124-6°) in 200 ml. CCl4 illuminated with a 250-w. lamp, and refluxed with 3.5 g. NBS and 0.15 g. Bz2O2 15 hrs. gave 3-hydroxy-3-phenyl-7-(dibromomethyl)phthalide (X), m. 166-70° (C6H6C6H14). X (2 g.) and 5% solution of Na2CO3 stirred 1 hr. at 80° gave 7-benzoyl-3-hydroxyphthalide (XI), m. 109-11° (C6H6C6H14). XI (816 mg.) added to 10 ml. III in 100 ml. H2O and the mixture stirred, refluxed 112 hrs., and filtered gave 7-phenyl-1,2,-8,9-tetraazaphenalene (XII), m. 292-3° (EtOH), methanesulfonate m. 256-7.5°. VI (1.86 g.) added to a stirred suspension of 0.07 g. MeONa in 100 ml. Me2SO, the mixture heated to 60°, treated with 2 ml. MeI at 50°, stirred 125 min. at 50-60°, and diluted with 500 ml. ice-cold H2O containing 0.5 g. NaHSO3 and 4 ml. AcOH gave 9-methyl-3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene, m. 289-93° (Me Cellosolve). VI (9.3 g.) and 10 drops H2O treated with 60 ml. POCl3 and the mixture refluxed 20 hrs. gave 3-chloro-1,2,8,9-tetraazaphenalene (XIII), decompose 270°. Similarly I prepared were: (X, R1, R2, R3 and m.p. given): Cl, Me, H, H (XIV), 253-5° (decomposition) (EtOH); Cl, Ph, H, H, 225-8° (EtOH); Cl, H, Ph, H, 278-88°. XIV (220 mg.) and 0.4 ml. NH4OH in 200 ml. EtOH hydrogenated over 0.8 g. 10% Pd-C gave 9-methyl-1,2,8,9-tetraazaphenalene (XV), m. 149-51°, HI salt m. 247-8°, methiodide m. 207-8.5° (EtOHEt2O). Similarly were prepared: XII and 9-phenyl-1,2,8,9-tetraazaphenalene (XVI), m. 168.5-70°. XIII (4.82 g.), 4 g. P, and 60 ml. 47% HI refluxed 18 hrs. gave IV, m. 294-8°. Similarly were prepared XV and XVI. VI (44.14 g.), 58.2 g. P2S5, and 356 ml. C5H5N stirred and refluxed 2.5 hrs. gave 35 g. 3-mercapto-1,2,8,9-tetraazaphenalene (XVII), m. 318-22° (aqueous Me Cellosolve or aqueous

HCONMe2). Similarly was prepared 9-methyl-3-thiono-2,3-dihydro-1,2,8,9-tetraazaphenalene, decompose 299-316°. XVII (4.04 g.) in 200 ml. Me Cellosolve and 200 ml. EtOH treated with 4 g. Raney Ni, and the mixture heated 4 hrs. to 100° gave IV. Similarly was prepared XV. XIII (1 g.), 15 ml. H2O and 85 ml. III stirred and refluxed 44 hrs. worked up and treated with 100 ml. 2N HCl3-hydrazino-1,2,8,9-tetraazaphenalene-2HCl (XVIII), m. 245-8° (decomposition) (aqueous HCl). Similarly prepared was 3-hydrazino-9-methyl-1,2,8,9-tetraazaphenalene-2HCl (XIX), decompose 260° (MeOH-Et2O). XVIII (28.7 g.), 800 ml. H2O and 400 ml. 10% aqueous CuSO4 heated 1 hr. to 100° gave IV. XIX (60 mg.) and 30 ml. phosphate buffer pH 7.2 kept 3 days at room temperature gave XV. XV (368 mg.), 145 mg. anhydrous NaOAc in 25 ml. AcOH treated dropwise with 320 mg. Br in 25 ml. AcOH and the mixture stirred 18 hrs. gave 3-bromo-9-methyl-1,2,8,9-tetraazaphenalene, m. 237-8° (EtOH). Similarly by bromination of the 3-unsubstituted derivs. the following I were prepared (X, R1, R2, R3, and m.p. given): Br, H, H, Br, >350°; Br, H, H, MeO, 291-4°; Br, H, H, BuO, 229-37°; Br, H, H, CO2H, 340°.

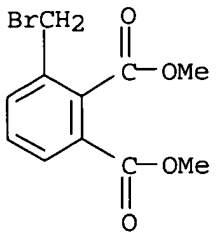
IT **14346-75-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14346-75-9 CAPLUS
CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)



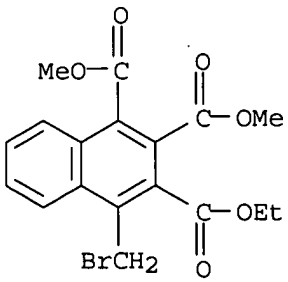
L3 ANSWER 189 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:512586 CAPLUS
DN 71:112586
TI Constitution and chemiluminescence. III. 5-[2-(Dialkylamino)vinyl]-2,3-dihydro-1,4-phthalazinediones
AU Gundermann, Karl D.; Schedlitzki, Dietmar
CS Tech. Univ. Clausthal, Clausthal, Fed. Rep. Ger.
SO Chemische Berichte (1969), 102(10), 3241-7
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA German
OS CASREACT 71:112586
GI For diagram(s), see printed CA Issue.
AB 2,3-(MeO2C)2C6H3Me was treated with N-bromosuccinimide and then NaCN to give 2,3-(MeO2C)2C6H3-CH2CH, which was catalytically reduced and treated with HCl to give 2,3-(MeO2C)2C6H3CH2CHO, acetalyzed and treated with N2H4 to give 3-(R-substituted)phthalic hydrazide (I, R = 1,3-dioxolanylmethyl). Treatment of the free aldehyde (I, R = CH2CHO) with R2NH gave I [R = (iso-Pr)2NCH:CH, (sec-Bu)2NCH:CH, (C5H11)2NCH:CH, or dicyclohexylaminovinyl]. I showed greater chemiluminescence during alkaline oxidation than I (R = dialkylamino), but less than I (R = NH2). They are much more easily hydrolyzed than I (R = NH2).

IT **24129-04-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24129-04-2 CAPLUS
CN 1,2-Benzenedicarboxylic acid, 3-(bromomethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

10803578



L3 ANSWER 190 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:491146 CAPLUS
DN 71:91146
TI Sulfoxonium ylide chemistry. III. Photochemistry of stable sulfoxonium ylides
AU Kishida, Yukichi; Hiraoka, Tetsuo; Ide, Junya
CS Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan
SO Chemical & Pharmaceutical Bulletin (1969), 17(8), 1591-7
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
OS CASREACT 71:91146
GI For diagram(s), see printed CA Issue.
AB Photochem. reaction of dimethylsulfoxonium 3-ethoxycarbonyl-2-phenylallylide gave diethyl p-terphenyl-2',5'-dicarboxylate in low yield. Irradiation of dimethylsulfoxonium 1,2-dicarbomethoxy-5-carbethoxy-4-phenyl-1,4-pentadien-3-ylide with an uv lamp afforded three products; 3-carbethoxy-1,2-dicarbomethoxy-4-methylnaphthalene (I) (37.5%), dimethyl 3-oxo-1,3-dihydronaphtho[1,2-c]furan-4,5-dicarboxylate (II) (0.39%), and dimethyl 3-oxo-1,3,4,5-tetrahydronaphtho[1,2-c]-furan-4,5-dicarboxylate (0.35%).
IT **19862-74-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19862-74-9 CAPLUS
CN 1,2,3-Naphthalenetricarboxylic acid, 4-(bromomethyl)-, 3-ethyl dimethyl ester (8CI) (CA INDEX NAME)



L3 ANSWER 191 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:491099 CAPLUS
DN 71:91099
TI Fluoroperhaloisopropylbenzenecarboxylic acids
IN Farah, Basil S.; Gilbert, Everett E.; Veldhuis, Benjamin
PA Allied Chemical Corp.
SO U.S., 4 pp.

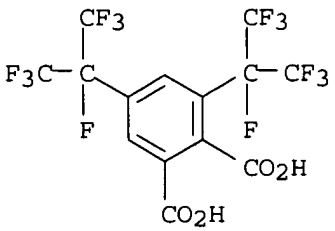
10803578

CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3462482	A	19690819	US 1966-583069	19660929
PRAI	US 1966-583069	A	19660929		

GI For diagram(s), see printed CA Issue.
AB The title compds. (I) show pesticidal activity. 4-[(F3C)2C(OH)]C6H4Me (129 g.) and 108 g. SF4 are sealed in a stainless steel bomb at -190° and warmed to room temperature overnight to yield 100 g. 4-(heptafluoro-isopropyl)toluene (II) b50 70°. CrO3 (200 g.) is added over 70 min. to 41.6 g. II, 1200 ml. HOAc and 152 ml. H2SO4. The temperature is held at 15° during the addition and then allowed to warm to room temperature to yield 4-(heptafluoroisopropyl)benzoic acid, m. 97-9°. The following I were similarly prepared [positions of CF(CF3)2, Me, CO2H groups(s) (- indicates no group present), % yield, b.p./mm. or m.p. given]; 2, 1,4, -, 66, 100°/110; 2,4, 1, -, 88, 68°/18; 3,5, 1,2, -, 53, 86°/20; 4,6, 1,3, -, 63, 188°/760; 2,5, 1,4, -, 60, -; 2, -, 1,4, 59, 175°; 2,4, -, 1 (III), 92, 103°; 3,5, -, 1,2, 20, 165°; 4,6, -, 1,3 (IV), 75, 245°; 2,5, -, 1,4, 64, 320°. II (43.5 g.) and 20 g. SOCl2 are mixed. The mixture is slowly heated to 167°. SOCl2 (20 g.) is added and after refluxing 6 hrs. at 82° the mixture is distilled to yield 24 g. 4-(heptafluoroisopropyl)benzoyl chloride (V), b10 75°. A mixture of 6.4 g. 4-chloroaniline and 85 ml. CCl4 is added to 7.7 g. of V in 25 ml. of CCl4. The mixture is cooled to room temperature and stirred 2.5 hrs. to yield 8.3 g. 4-(heptafluoro-isopropyl)benz-4-chloroanilide, m. 141-1.5°. English broadleaf bean plants are sprayed 10 sec. at 0.6 ml./sec. with 2 lb. of III/100 gal. of 1:1 acetone-H2O. The mortality of adult female pea aphids is 100% 3 days after infesting the sprayed plants. In a nematode toxicity test 5 ml. of 1% aqueous IV gives complete kill of nematodes in 3 days. A wettable powder containing 25% V shows fair ovicidal activity against two-spotted spider mites on cranberry bean plants.

IT **24062-99-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24062-99-5 CAPLUS
CN Phthalic acid, 3,5-bis[tetrafluoro-1-(trifluoromethyl)ethyl]- (8CI) (CA INDEX NAME)



L3 ANSWER 192 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:115190 CAPLUS
DN 70:115190
TI Preparation of new 1,2,8,9-tetraazaphenalenes
IN Doebel, Karl J.; Francis, John E.
PA Geigy, J. R., A.-G.

10803578

SO S. African, 37 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 1

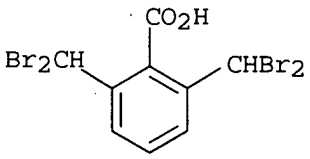
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 6705856		19680723		
	CH 515909			CH	
	DE 1695038			DE	
	DE 1695039			DE	
	FR 7210			FR	
	FR 7211			FR	
	GB 1204522			GB	
	GB 1208114			GB	
	US 3422105		19690000	US	
	US 3535320		19700000	US	
	US 3539567		19700000	US	
	US 3560499		19710000	US	
	US 3560500		19710000	US	
	US 3562268		19710000	US	
	US 3562271		19710000	US	
	US 3575976		19710000	US	
	US 3578665		19710000	US	
	US 3691165		19720000	US	
	US 3761493		19730000	US	
PRAI	US		19661003		

GI For diagram(s), see printed CA Issue.

AB Title compds. (I), their addition salts and quaternary ammonium compds., having hypotensive and sedative properties, and useful as cardiovascular agents, were prepared Thus, a mixture of 81 g. 3-methylphthalic anhydride, 182 g. N-bromosuccinimide and 80 mg. Bz2O2 in 15 l. CCl4 is irradiated under reflux 24 hrs. to give the dibromomethyl analog (II), m. 93-5° (Et2O-hexane). A suspension of 80 g. II in 500 ml. EtOH is treated with a solution of 100 ml. N2H4.H2O (100%) in 100 ml. H2O under stirring and refluxing 88 hrs. and the mixture worked up to give 3-hydroxy-1,2,8,9-tetraazaphenalene (I) (R1 = R2 = H, R3 = OH) (Ia), m. >350° [HCONMe2 (DMF)]. A mixture of 9.3 g. of this with 10 drops H2O and 60 ml. POCl3 is refluxed 20 hrs. and worked up to give the 3-chloro analog (Ib); HCl salt m. 270° (decomposition) (EtOH). A mixture of 4.82 g. of this salt, 4 g. red P, and 60 ml. 47% HI is refluxed 18 hrs. to yield 1,2,8,9-tetraazaphenalene (III), m. 294-8°. Similarly is prepared I (R1 = Me, R2 = R3 = H) (IIIa) m. 149-51° (benzene-hexane); HI salt m. 247-8°. A mixture of 44.14 g. I (R1 = R2 = H, R3 = NHNH2), 58.2 g. P2S5, and 356 ml. dry pyridine is refluxed 2.5 hrs. with stirring and worked up to give 3-mercapto-1,2,8,9-tetraazaphenalene (IV), m. 318-22° (aqueous DMF). Similarly is prepared I (R1 = Me, R2 = H, R3 = SH), m. 299-316° [Me Cellosolve (MEC)] from I (R1 = Me, R2 = H, R3 = OH) (IVa). A solution of 4.04 g. IV in 200 ml. MEC and 200 ml. EtOH is treated with 20 g. Raney Ni and heated 4 hrs. on a steam bath to give III. The yellow solid (1 g.), obtained in the reaction of 9.3 g. Ia with 60 ml. POCl3 and 10 drops H2O, is suspended in 15 ml. H2O containing 85 ml. N2H4.H2O (100%), refluxed 44 hrs., and worked up to give 3-hydrazino-1,2,8,9-tetraazaphenalene (V); di-HCl salt m. 245-8° (dilute HCl) salt m. 245-8° (dilute HCl). A solution of 28.7 g. V.2HCl in 800 ml. H2O is heated 1 hr. at 100° with 400 ml. 10% aqueous CuSO4 and the mixture made strongly alkaline to give III. A mixture of 1.86 g. Ia and 0.07 g. NaOMe in 100 ml. dry Me2SO is stirred at 60°, 2 ml. MeI added, and the mixture stirred 3 hrs. at 50-60° to give IVa, m. 289-93° (MEC). A mixture of PCl5, POCl3, and IVa is refluxed 2 hrs. with stirring to give I

(R1 = Me, R2 = H, R3 = Cl) (Va), m. 253-5° (EtOH). Similarly are prepared I (R1 = Ph, R2 = H, R3 = Cl), m. 225-8° (EtOH); and (R1 = H, R2 = Ph, R3 = Cl), m. 278-88°. Va (220 mg.), 0.4 ml. concentrated NH4OH, 0.8 g. 10% Pd/C and 200 ml. EtOH is stirred in a H atmospheric to give IIIa, m. 149-51° (benzene-hexane). Similarly are prepared 9-phenyl-1,2,8,9-tetraazaphenalene, m. 168.5-70° (benzene); and 7-phenyl-1,2,8,9-tetraazaphenalene, m. 292-3° (EtOH); methanesulfonate m. 256-7.5°. A mixture of I (R1 = Me, R2 = H, R3 = SH) and N2H4.H2O (100%) in H2O is stirred at reflux 20 hrs. and worked up to yield I.HCl (R1 = Me, R2 = H, R3 = NHNH2), m. 260° (decomposition) (MeOHEt2O). A suspension of 60 mg. of this in 30 ml. phosphate buffer (pH 7.2) is left in the dark 3 days to give IIIa; methiodide m. 207-8.5° (MeOH-Et2O). To a solution of 0.37 g. IIIa and 0.16 g. NaOAc in 25 ml. HOAc is added dropwise 0.32 g. Br in 25 ml. HOAc and the solution stirred 18 hrs. to give 3-bromo-1,2,8,9-tetraazaphenalene, m. 237-8° (EtOH). II (40 g.) is added slowly to a hot solution of 500 ml. 2N NaOH, and the solution acidified after 10 min. to give 7-carboxy-3-hydroxyphthalide, m. 165.5-8.5° (H2O); 5.82 g. of this, 3.6 ml. PhNHNH2, and 100 ml. HOAc is refluxed 18 hrs. to give 8-carboxy-2-phenyl-1(2H)-phthalazinone, m. 197-8° (benzene); Et ester m. 150-1° (EtOH). This (11.76 g.), 40 ml. N2H4.H2O (100%) and 160 ml. MEC is refluxed 25 hrs. and worked up to give 9-phenyl-(2H)(9H)-1,2,8,9-tetraazaphenalen-3-one, m. 255-7° (MEC). Similarly is prepared the 7-Ph isomer, m. >350° (MEC). Heating a mixture of 32.5 g. 3-benzoylphthalic acid, 85 ml. N2H4.H2O and 145 ml. H2O 18 hrs. gives 8-carboxy-4-phenyl-1(2H)-phthalazinone, m. 257-9° (HOAc), Me ester m. 198-202°. Br (75 g.) in 350 ml. CCl4 is added dropwise during 30 min. at reflux temperature to a solution of 36 g. 2,6-dimethylbenzoic acid in 120 ml. CCl4 under stirring and irradiation to yield 90% 2,6-bis(dibromomethyl)benzoic acid, m. 203-6° (decomposition). This (9.3 g.) is added gradually to a stirred solution of 20 ml. N2H4.H2O (100%) in 180 ml. H2O and the solution refluxed 95 hrs. to give III.

IT **14346-75-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14346-75-9 CAPLUS
CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)



L3 ANSWER 193 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:115177 CAPLUS
DN 70:115177
TI 1,2,8,9-Tetraazaphenalenes
IN Doebel, Karl J.; Francis, John E.
PA Geigy Chemical Corp.
SO U.S., 8 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3429882	A	19690225	US 1968-715525	19680325

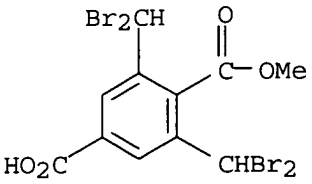
10803578

PRAI US 1968-715525 A 19680325
GI For diagram(s), see printed CA Issue.
AB 1,2,8,9-Tetraazaphenalenes (I) were prepared and used as cardiovascular agents. Thus, a solution of 17 g. 2,6-Me2C6H3CO2H in 1.2 l. CCl4 was refluxed, 75 g. Br in 350 ml. CCl4 added dropwise and the mixture refluxed and irradiated until HBr ceased to evolve, and worked up to give 2,6-bis(dibromomethyl)benzoic acid (II), m. 203-6°. II was converted into 3-hydroxy-7-formylphthalide (III), m. 127-33°, by treating with 5% Na2CO3 followed by acidifying with concentrated HCl. III (11.7 g.) was suspended in 390 ml. H2O, added slowly to 47 ml. N2H4.H2O, and the mixture refluxed 66 hrs., filtered hot, and cooled to give 55% I (R1 = R2 = R3 = H) (IV), m. 287-93°. Recrystn. from H2O, absolute EtOH, and H2O successively gave a pure sample, sublimed 190-240°. III (6 g.) was added to 100 ml. N2H4.H2O, and the mixture refluxed 30 min. and worked up to give 8-formyl-1(2H)-phthalazinone hydrazone (V), m. 235-7°. To a solution of 10 ml. 100% N2H4.H2O in 100 ml. H2O, 0.94 g. V was added, and the mixture refluxed 24 hrs., filtered hot, and cooled to give 0.7 g. IV, also prepared by heating 4.04 g. 3-thiono-2,3-dihydro-1,2,8,9-tetraazaphenalene (VI) in 200 ml. Me Cellosolve and 200 ml. EtOH with 20 g. Raney Ni. VI, m. 318-22°, was prepared by refluxing 3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene (VII) with P2S5 and pyridine. VII, m. 350°, was prepared by refluxing 3-(dibromomethyl)phthalic anhydride (VIII) suspension in EtOH with N2H4.H2O. VIII, m. 93°, was prepared by irradiating a mixture of 3-methylphthalic anhydride, N-bromosuccinimide, Bz2O2, and CCl4. I (R1 = Me, R2 = R3 = H) (IX), m. 145-7° (HI salt m. 247-8°; MeI salt m. 207-8.5°), was prepared by treating 3-thiono-9-methyl-1,3-dihydro-1,2,8,9-tetraazaphenalene (X), m. 299-316° (decomposition), with Raney Ni in EtOH. X was prepared from 3-oxo-9-methyl-1,2,8,9-tetraazaphenalene. IX, m. 149-51°, was also prepared by heating a mixture of I (R1 = Me, R2 = Cl, R3 = H), m. 253-5°, with P and HI. IV was also prepared by treating 3-hydrazino-1,2,8,9-tetraazaphenalene-2HCl, m. 245-8°, with 10% aqueous CuSO4. I (R1 = Ph, R2 = R3 = H), m. 168.5-70°, was prepared by treating I (R1 = Ph, R2 = Cl, R3 = H) (XI), m. 225-8°, with P and HI. XI was prepared by refluxing 3-oxo-9-phenyl-2,3-dihydro-1,2,8,9-tetraazaphenalene (XII), m. 254-6°, with PCl5 and POCl3. XII was prepared by refluxing a mixture of 8-carboxy-2-phenyl-1(2H)-phthalazinone (XIII), m. 197-8°, with SOCl2 in PhCl. XIII was prepared by treating VII with hot 2N NaOH followed by acidification. I (R1 = R2 = H, R3 = 5-OMe) (XIV), m. 291-4° (methanesulfonate m. 255-7°), was prepared in 15.5% yield by treating 3-hydroxy-5-methoxy-7-formylphthalide, m. 174-5° [obtained from 4-methoxy-2,6-bis(dibromomethyl)-benzoic acid, m. 201-2°], with N2H4.H2O. I (R1 = R2 = H, R3 = 5-Br), m. 350° (methanesulfonate m. 264-8°), was prepared by treating 3-hydroxy-5-bromo-7-formylphthalide (XV) with N2H4.H2O. XV, m. 187-9°, was prepared from 4-bromo-2,6-bis(dibromomethyl)benzoic acid, m. 220-1°. I (R1 = R2 = H, R3 = 5-CO2H), m. 340°, was prepared by treating Me 4-carboxy-2,6-bis(dibromomethyl)benzoate, m. 211.5-13°, with aqueous Na2CO3. IV on nitration with HNO3-H2SO4 gave the 4,6-dinitro derivative 7-Phenyl-1,2,8,9-tetraazaphenalene, m. 292-3°, was prepared by treating 3-hydroxy-7-benzoylphthalide, m. 109-11°, prepared from 3-hydroxy-3-phenyl-7-dibromomethylphthalide, m. 166-70°, with N2H4.H2O. XIV was refluxed with 48% HBr to give I (R1 = R2 = H, R3 = 5-OH) HBr salt, m. 340°. IV was converted into I (R1 = R2 = H, R3 = 4-Br) HCl salt, m. 258-60°, by successive treatment with N-bromosuccinimide, NaOH, and 6N HCl. I (R1 = R2 = H, R3 = 5-OBu), m. 229-37°, was prepared by treating 4-butoxy-2,6-bis(dibromomethyl)benzoic acid, m. 166-71°, with N2H4.H2O. I (R1 = R2 = H, R3 = 4-Cl), m. 260-3°, was prepared by treating IV with N-chlorosuccinimide in 50% H2SO4. I (R1 = PhCH2, R2 = R3 = H) was prepared

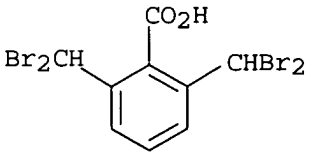
by treating IV with NaOMe and PhCH2Br. The m.p. of IV HCl, maleate, and methanesulfonate, and MeI, EtI, and iso-PrI salts were 254-7, 150-1, 288-93, 268-9, 260-2, and 256°, resp. I (R1 = R3 = H, R2 = Ph) methanesulfonate, m. 256-7.5°, was also prepared Spectral data (uv, ir, N.M.R.) were given for some of the compds.

IT **14346-63-5P 14346-75-9P 15562-75-1P 15562-76-2P 15562-77-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

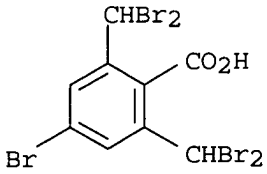
RN 14346-63-5 CAPLUS
CN Terephthalic acid, 2,6-bis(dibromomethyl)-, 1-methyl ester (8CI) (CA INDEX NAME)



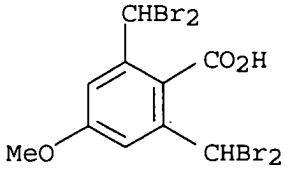
RN 14346-75-9 CAPLUS
CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)



RN 15562-75-1 CAPLUS
CN Benzoic acid, 4-bromo-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)

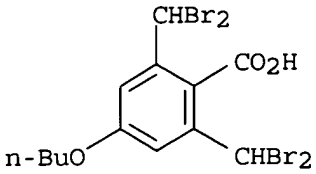


RN 15562-76-2 CAPLUS
CN p-Anisic acid, 2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)

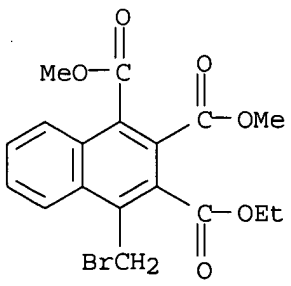


RN 15562-77-3 CAPLUS
CN Benzoic acid, 4-butoxy-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)

10803578



L3 ANSWER 194 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1968:467047 CAPLUS
DN 69:67047
TI The photochemistry of a stable sulfoxonium ylide
AU Kishida, Yukichi; Hiraoka, Tetsuo; Ide, Junya
CS Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan
SO Tetrahedron Letters (1968), (9), 1139-42
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB Irradiation of the sulfoxonium ylide PhC(:CHCO2Et)C-[C(CO2Me):CHCO2Me]S+OMe2 (I), in a 1:2 EtOH-tetrahydrofuran mixture for 2 hrs. with a uv 450-w lamp and chromatog. of the products on silica gel yielded 37.5% naphthalene derivative (II), m. 106-7°. II reduced with LiAlH4 gave a triol, m. 168-9°, brominated with PBr3 to a tribromide, m. 193-4°. Reduction of the tribromide with LiAlH4 in tetrahydrofuran gave 1,2,3,4-tetramethylnaphthalene. II hydrolyzed with NaOH, followed by treatment with HCl gave a mixture of carboxylic acid anhydrides, decarboxylated by heating with Cu powder in quinoline to give 1-methylnaphthalene. The residual product after separation of II was chromatographed on silica gel impregnated with AgNO3 to yield 0.39% III, m. 180.5-2.0°. II brominated with N-bromosuccinimide (NBS) in CCl4 gave a monobrominated compound, m. 109-11°, heated at 200° to yield III. The 3rd product obtained in 0.35% yield from I was IV, m. 165-7°. IV brominated with NBS in CHCl3 and the product dehydrobrominated with NEt3 gave III.
IT **19862-74-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19862-74-9 CAPLUS
CN 1,2,3-Naphthalenetricarboxylic acid, 4-(bromomethyl)-, 3-ethyl dimethyl ester (8CI) (CA INDEX NAME)



L3 ANSWER 195 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:65519 CAPLUS
DN 66:65519
TI New 1,2,8,9-tetraazaphenalenes

10803578

PA Geigy, J. R., A.-G.
SO Neth. Appl., 18 pp.
CODEN: NAXXAN
DT Patent
LA Dutch
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	NL 6604484	A	19661006	NL 1966-4484	19660404
	SE 317387	B	19691117	SE 1966-4486	19660404
	SE 318284	B	19691208	SE 1968-11955	19660404
	NO 118492	B	19700105	NO 1966-162451	19660404
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	IL 25525	A1	19700420	IL 1966-25525	19660404
	SE 323688	B	19700511	SE 1966-4485	19660404
	SE 323689	B	19700511	SE 1966-4487	19660404
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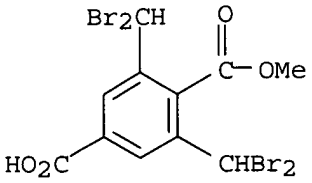
	SE 350262	B	19721023	SE 1970-2423	19660404
	SE 350263	B	19721023	SE 1970-2424	19660404
	BE 679045	A	19661005	BE 1966-679045	19660405
	BE 679046	A	19661005	BE 1966-679046	19660405
	BE 679047	A	19661005	BE 1966-679047	19660405
	CH 475994	A	19690731	CH 1966-475994	19660405
	CH 478807	A	19690930	CH 1966-478807	19660405
	CH 481122	A	19691115	CH 1966-481122	19660405
	CH 482698	A	19691215	CH 1966-482698	19660405
	CH 483432	A	19691231	CH 1966-483432	19660405
	US 3539567	A	19701110	US 1968-729487	19680423
	US 3624108	A	19711130	US 1969-889795	19691215
	NO 121785	B	19710413	NO 1969-5042	19691219
	US 3761493	A	19730925	US 1970-81114	19701015
PRAI	US 1965-445762	A	19650405		
	US 1966-539303	A2	19660401		
	NO 1966-162450	A	19660404		
	US 1966-583980	A2	19661003		
	US 1968-729487	A3	19680423		
	US 1969-889795	A3	19691215		

AB cf. preceding abstrs. The preparation of the title compds., their acid addition salts, and quaternary ammonium compds. is described. The products are suitable pharmaceuticals, in particular valuable blood-pressure reducing agents. Thus, 11.7 g. 3-hydroxy-7-formylphthalide (I), m. 127-33°, in 390 ml. H2O was slowly added with stirring to a solution of 47 ml. N2H4.H2O and the mixture refluxed 66 hrs., treated with C, filtered warm, and cooled to give 55% 1,2,8,9-tetraazaphenalene (II), sublimes 190-240°, decomposed 294-8° (absolute EtOH and H2O). I, m. 127-33°, was obtained in a 82% yield from 600 ml. 5% Na2CO3 solution and 37.2 g. 2,6-bis(α,α-dibromomethyl)benzoic acid (III), m. 203-6°, while III was prepared from 36 g. 2,6-dimethylbenzoic acid and 75 g. Br in 350 ml. CCl4 in a 90% yield by boiling the mixture 30 min. III (9.3 g.) added to 20 ml. N2H4.H2O in 180 ml. H2O with stirring and the mixture refluxed 95 hrs. gave 2.17 g. II, m. 294-8° (decomposition). II was also prepared from 150 mg. 8-formyl-1-(2H)-phthalazinone (IV) and 130 ml. HCONMe2 whereby IV was obtained from 6 g. I and 100 ml. 100% N2H4.H2O and 65 ml. H2O by refluxing the mixture 30 min. to give 3.25 g. IV of which a small amount sublimed 120°/0.05 mm.; IV m. 235-7°. IV (0.94

g.) in 10 ml. $N_2H_4.H_2O$ and 100 ml. H_2O refluxed 24 hrs. gave 0.70 g. II. II (170 mg.) dissolved in 20 ml. 6N HCl and the mixture concentrated and worked up gave 0.3 g. II.HCl, m. 254-7°, decomposed 293-7°. II (5.1 g.) and 5 ml. $MeSO_3H$ in 125 ml. MeOH gave after stirring 20 min. at 60° and treatment of the mother liquor with Et_2O 6.7 g. 1,2,8,9-tetraazaphenalene methanesulfonate, m. 288-93° (HCONMe2). II (170 mg.) in 10 ml. EtOH and 117 mg. maleic acid in 10 ml. EtOH gave 189 mg. II maleate, m. 150-1° (EtOH). A mixture of 266 mg. II, 5 ml. MeI, and 24 ml. absolute MeOH was heated 23 hrs. to give 475 mg. II.MeI, m. 279-81° (MeOH). Similarly was prepared II.EtI, m. 260.2° (EtOH). Reflux of 10 ml. iso-PrI, 150 ml. iso-PrOH, and 3.4 g. II 48 hrs. gave II.iso-PrI, m. 256-7° (MeOH-Et_2O). $AgNO_3$ (35 mg.) was dissolved in H_2O, 10 ml. EtOH added, 2 ml. 0.1N NaOH and then 62.4 mg. quaternary II.MeI added, and the mixture stirred at 50° to give 29 mg. 9-methyl-1,2,8,9-tetraazaphenalene, m. 190-200° (decomposition). Heating a mixture of 1.7 g. II, 1.2 ml. Me_2SO_4, and 50 ml. EtOH 24 hrs. gave 9-methyl-1,2,8,9-tetraazaphenalene methosulfate, m. 202-4° (MeOH-Et_2O). The latter treated with 5% aqueous $NaHCO_3$ solution, the suspension obtained extracted with $CHCl_3$, and the exts. extracted with 3N HCl gave 9-methyl-1,2,8,9-tetraazaphenalene-HCl, m. 276-8° (EtOH-Et_2O). Other compds. prepared were: 1,9-dimethyl-1,2,8,9-tetraazaphenalene bisulfate, m. 337-40° (MeOH-H_2O); 9-methyl-1,2,8,9-tetraazaphenalene-MeI, m. 313-14° (HCONMe2); 5-methoxy-1,2,8,9-tetraazaphenalene, m. 291-4° (EtOH-EtOAc) (decomposition) (15.5% yield); 5-methoxy-1,2,8,9-tetraazaphenalene methanesulfonate, m. 255-7° (MeOH) (86% yield); 5-hydroxy-1,2,8,9-tetraazaphenalene-HBr, m. >340°; 5-bromo-1,2,8,9-tetraazaphenalene, m. >350°; hydrochloride m. >340°; methanesulfonate m. 264-8° (decomposition). Reflux of a mixture of 27.8 g. 4-butoxy-2,6-bis(bromomethyl)benzoic acid, 130 ml. $N_2H_4.H_2O$, and 1300 ml. H_2O 22 hrs. with stirring gave 5-butoxy-1,2,8,9-tetraazaphenalene, m. 229-37° (EtOAc). Similarly was obtained 5-carboxy-1,2,8,9-tetraazaphenalene, m. >340°, from Me 4-carboxy-2,6-bis(bromomethyl)benzoate treated with 5% aqueous $NaHCO_3$ solution [TABLE OMITTED]

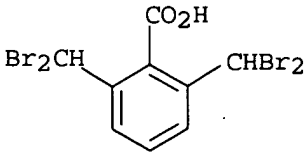
IT **14346-63-5P 14346-75-9P 15562-75-1P 15562-76-2P 15562-77-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14346-63-5 CAPLUS
CN Terephthalic acid, 2,6-bis(dibromomethyl)-, 1-methyl ester (8CI) (CA INDEX NAME)

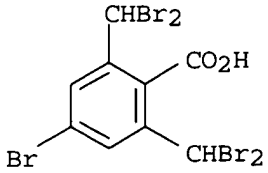


RN 14346-75-9 CAPLUS
CN Benzoic acid, 2,6-bis(dibromomethyl)- (8CI, 9CI) (CA INDEX NAME)

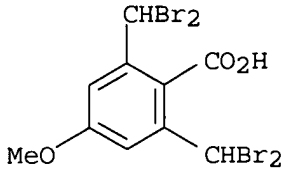
10803578



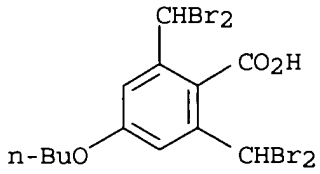
RN 15562-75-1 CAPLUS
CN Benzoic acid, 4-bromo-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)



RN 15562-76-2 CAPLUS
CN p-Anisic acid, 2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)



RN 15562-77-3 CAPLUS
CN Benzoic acid, 4-butoxy-2,6-bis(dibromomethyl)- (8CI) (CA INDEX NAME)



L3 ANSWER 196 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:65517 CAPLUS
DN 66:65517
TI New 1,2,8,9,-tetraazaphenalenes
PA Geigy, J. R., A.-G.
SO Neth. Appl., 22 pp.
CODEN: NAXXAN
DT Patent
LA Dutch
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	NL 6604482	A	19661006	NL 1966-4482	19660404
	SE 317387	B	19691117	SE 1966-4486	19660404
	SE 318284	B	19691208	SE 1968-11955	19660404
	NO 118492	B	19700105	NO 1966-162451	19660404
	NO 118493	B	19700105	NO 1966-162452	19660404

	IL 25525	A1	19700420	IL 1966-25525	19660404
	SE 323688	B	19700511	SE 1966-4485	19660404
	SE 323689	B	19700511	SE 1966-4487	19660404
	IL 25526	A1	19700521	IL 1966-25526	19660404
	IL 25524	A1	19700617	IL 1966-25524	19660404
	DK 119313	B	19701214	DK 1966-1747	19660404
	DK 119504	B	19710118	DK 1966-1746	19660404
	NO 121495	B	19710308	NO 1966-162450	19660404
	DK 120240	B	19710503	DK 1966-1748	19660404
	SE 350262	B	19721023	SE 1970-2423	19660404
	SE 350263	B	19721023	SE 1970-2424	19660404
	BE 679045	A	19661005	BE 1966-679045	19660405
	BE 679046	A	19661005	BE 1966-679046	19660405
	BE 679047	A	19661005	BE 1966-679047	19660405
	CH 475994	A	19690731	CH 1966-475994	19660405
	CH 478807	A	19690930	CH 1966-478807	19660405
	CH 481122	A	19691115	CH 1966-481122	19660405
	CH 482698	A	19691215	CH 1966-482698	19660405
	CH 483432	A	19691231	CH 1966-483432	19660405
	US 3539567	A	19701110	US 1968-729487	19680423
	US 3624108	A	19711130	US 1969-889795	19691215
	NO 121785	B	19710413	NO 1969-5042	19691219
	US 3761493	A	19730925	US 1970-81114	19701015
PRAI	US 1965-445762	A	19650405		
	US 1966-539303	A2	19660401		
	NO 1966-162450	A	19660404		
	US 1966-583980	A2	19661003		
	US 1968-729487	A3	19680423		
	US 1969-889795	A3	19691215		

GI For diagram(s), see printed CA Issue.

AB cf. following abstract The preparation of 3-hydroxy-1,2,8,9-tetraazaphenalene (I), 3-mercapto-1,2,8,9-tetraazaphenalene (II) and the corresponding 3-oxo- or 3-thioxo-2,3-dihydro-1,2,8,9-tetraazaphenalenes is described. The products are suitable pharmaceuticals, in particular valuable bloodpressure-reducing agents. Thus, a mixture of 81 g. 3-methylphthalic anhydride, 182 g. N-bromosuccinimide, 40 mg. Bz2O2, and 1500 ml. CCl4 was refluxed until red to litmus, 40 ml. Bz2O2 added, the reaction continued 24 hrs. with stirring and irradiation, the mixture cooled, succinimide filtered off, the filtrate evaporated to dryness, the residue passed into warm Et2O, treated with C, and filtered, hexane added to the filtrate, and the filtrate cooled to give 72% α,α-dibromo-3-methylphthalic anhydride (III), m. 93-5° (Et2O-hexane). To a suspension of 80 g. III in 500 ml. EtOH was added dropwise with stirring and cooling 100 ml. N2H4.H2O and 100 ml. H2O, the mixture refluxed 88 hrs. with stirring, cooled, and filtered, the mother liquor evaporated to dryness, the residue in 500 ml. glacial AcOH refluxed 18 hrs. and cooled, a second portion filtered off, and the combined products washed with H2O and EtOH and dried to give 55% crude I. This was recrystd. from HCONMe2 to give yellow powdered I, microcryst. at 220-70°, m. >350°. To a solution of 20 ml. SOCl2 in 100 ml. PhCl was added with vigorous stirring 15.2 g. 8-carboxy-1(2H)-phthalazinone (IV), the mixture refluxed with the exclusion of moisture 4 hrs. and cooled, and the precipitate rapidly filtered off, washed with C6H6, and dried in vacuo over P2O5 to give 16.5 g. product, of which 3.98 g. was added with stirring to a solution of 10 ml. 100% N2H4.H2O, 10 ml. H2O, and 25 ml. EtOH and the mixture boiled 48 hrs., filtered, and washed with H2O and EtOH to give 2.31 g. dry I, m. 348°. α,α-Dibromomethylphthalic anhydride, m. 90.5-93° (40 g.), was added to 500 ml. warm 2N NaOH, the solution acidified after 10 min. with concentrated HCl and further heated 0.5 hr. at 80°, the solution concentrated and dried, the residue passed into 600 ml. warm H2O, treated with C, and

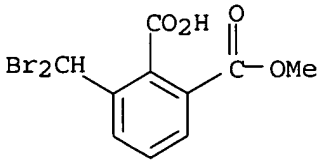
filtered, and the filtrate kept 3 days at 5° to give 88% 3-hydroxy-7-carboxyphthalide (V), m. 165.5-6.5° (H2O). A mixture of 30.2 g. V, 50 ml. 100% N2H4H2O, and 100 ml. H2O refluxed 16 hrs. gave 99% IV, m. 303.5-306° (glacial AcOH). IV was also prepared from 20 ml. N2H4.H2O in 200 ml. CHCl3 and 8 g. α,α-dibromo-3-methylphthalic anhydride in ml. 50 CHCl3 refluxed 18 hrs. Workup gave IV, m. 297-304° (glacial AcOH). I was also prepared by refluxing 110 hrs. 1.02 g. 8-carbomethoxy-1(2H)-phthalazinone (VI), 5 ml. 100% N2H4.H2O, and 20 ml. absolute EtOH to yield 84% I, m. 350°. A solution of 7.6 g. 8-carboxy-1(2H)-phthalazinone in 100 ml. absolute MeOH and .apprx.0.1 mole of a diazo solution in Et2O was stirred overnight at room temperature to give 6.25 g. VI, m. 207-9° (MeOH). Similarly was prepared 0.82 g. I, m. 350°, from 1.11 g. 3-methoxy-7-carbomethoxyphthalide, 4 ml. 100% N2H4.H2O, and 10 ml. absolute EtOH refluxed 94 hrs. Other starting compds. used were 3-bromo-7-chlorocarbonylphthalide, 8-carbethoxy-1(2H)-phthalazinone, and 2-dibromomethyl-6-carbomethoxybenzoic acid (preparation described). A mixture of 58.2 g. P2S5 and 44.14 g. I in 356 ml. absolute pyridine was refluxed 2.5 hrs., the liquid cooled and poured into 1 l. ice-cold saturated NaCl solution, and the mixture stirred 1.5 hrs. filtered, washed with H2O, and dried at 100° to give 35 g. product, m. 298-320° (decomposition). Recrystn. from a mixture of Me Cellosolve and H2O and from HCONMe2-H2O gave powdered II, m. 318-322° (preheated melt-block of 250°). Refluxing 1.16 g. 2-methyl-8-carbethoxy-1(2H)-phthalazinone, 5 ml. N2H4.H2O, and 20 ml. Me Cellosolve 26 hrs. and workup gave 386 mg. 9-methyl-3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene (VII) m. 305-6° (Me Cellosolve). Carbethoxy-1(2H)-phthalazinone (3.0 g.) dissolved in 11 ml. 2N NaOH, 60 ml. H2O added, and 4.2 ml. Et2SO4 added dropwise, the solution stirred 60 hrs. at room temperature while the pH was adjusted to 4 and stirred another 2 hrs. at room temperature, the product extracted with CHCl3, the extract dried and concentrated, and the residue distilled gave 2-ethyl-8-carbethoxy-1(2H)-phthalazinone. The latter (1.6 g.) was suspended in 5.7 ml. N2H4.H2O and 23 ml. Me Cellosolve and the mixture refluxed 96 hrs. to give 0.5 g. 9-ethyl-3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene, m. 218-19° (H2O). A mixture of 11.76 g. 2-phenyl-8-carbethoxy-1-(2H)-phthalazinone, 40 ml. 100% N2H4.H2O, and 100 ml. Me Cellosolve gave after 25 hrs. reflux 4.44 g. 9-phenyl-2-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene (VIII), m. 255-7° (Me Cellosolve). A mixture of 2.6 g. VIII, 2.5 g. P2S5, and 15 ml. absolute pyridine refluxed 2.5 hrs. and poured into 200 ml. ice-cold NaCl solution gave 1.68 g. pure 9-phenyl-3-thioxo-2,3-dihydro-1,2,8,9-tetraazaphenalene, m. 232°-4° (EtOH). A mixture of 0.7 g. NaOMe in 100 ml. anhydrous Me2SO and 1.80 g. 3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene was stirred at 60° until a red solution was formed, the mixture cooled to 50°, 1 ml. MeI added and after 20 min. another ml. MeI, and the mixture stirred 125 min. at 50-60°, poured into 500 ml. ice-water containing 0.5 g. NaHSO4 and 4 ml. glacial AcOH, kept overnight, and filtered to give 1.2 g. 9-methyl-3-oxo-2,3-dihydro-1,2,8,9-tetraazaphenalene (Me Cellosolve), identical to VII.

IT **14346-58-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14346-58-8 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3-(dibromomethyl)-, 1-methyl ester (9CI) (CA INDEX NAME)

10803578



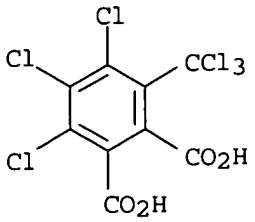
L3 ANSWER 197 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1961:29731 CAPLUS
DN 55:29731
OREF 55:5856h-i,5857a-b
TI Ring-substituted derivatives of α,α,α,2,3,4-hexachlorotoluene
IN Molotsky, Hyman M.
PA Velsicol Chemical Corp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2946817		19600726	US	
	GB 845036			GB	

AB To 610 g. hexachlorocyclopentadiene (I) at 110° 95 g. CH.tplbond.CCH2Cl was added in 4 hrs., and the temperature was allowed to rise to 145° in 16 hrs. to give an adduct (II), b1.3 122°, n20D 1.5665. II (90 g.) was added in 0.5 hr. to 220 g. I at 220° to yield after 1 hr. at 220-35° crude chloromethyl-α,α,α,2,3,4-hexachlorotoluene (III), b0.8 155-8°, m. 91-2.5°. III was hydrolyzed by 0.1N H2SO4 to chloromethyl-2,3,4-trichlorobenzoic acid. (.tplbond.CCH2Cl)2 (121 g.) was added to 405 g. I at 170°, and the mixture was refluxed at 170-80° for 8 hrs. to yield a crude adduct (IV), b1.6 155-7°. IV (106 g.) was refluxed with 206 g. I at 240-8° for 2.5 hrs. to yield 5,6-dichloromethyl-α,α,α,2,3,4-hexachlorotoluene, b2 17°, n20D 1.6180. I-PhC.tplbond.CH adduct (150 g.) was refluxed for 1 hr. at 230-50° to yield phenyl-α,α,α,2,3,4-hexachlorotoluene (V), b1.4 200°, n25D 1.6402. CH.tplbond.CCO2Et (76.4 g.) was added to 273 g. I at 140° to give after 6 hrs. at 140-50° an adduct (VI), b0.2 116.5°, n20D 1.5420. VI (100 g.) in 200 g. I was refluxed for 3 hrs. at 240-50° to yield carbethoxy-α,α,α,2,3,4-hexachlorotoluene. CH.tplbond.CCH2OH (45 g.) was added to 273 g. I to yield after 7 hrs. at 150-60° an adduct, b1.7 145°, m. 86.5-7.5°, which, on refluxing with excess Ac2O for 4 hrs., gave an acetate (VII), b1.0 130-1°, n20D 1.5330. Refluxing 100 g. VII with 200 g. I for 3 hrs. at 270° yielded acetoxymethyl-α,α,α,2,3,4-hexachlorotoluene, b0.5 154-6°, n20D 1.5855. A 0.4% aqueous dispersion of V (used as a 10% wettable powder) was insecticidal in 48 hrs.: Mexican bean beetle, 100% (also for 0.2%); Southern army worm, 100%; pea aphid, 89.6%.

IT **109069-49-0**, Phthalic acid, 3,4,5-trichloro-6-(trichloromethyl)- (preparation of)
RN 109069-49-0 CAPLUS
CN Phthalic acid, 3,4,5-trichloro-6-(trichloromethyl)- (6CI) (CA INDEX NAME)

10803578



L3 ANSWER 198 OF 198 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1960:97315 CAPLUS
DN 54:97315
OREF 54:18396b-e
TI Trimerization of hexafluoro-2-butyne
AU Harris, J. F., Jr.; Harder, R. J.; Sausen, G. N.
CS E. I. du Pont de Nemours & Co., Inc., Wilmington, DE
SO Journal of Organic Chemistry (1960), 25, 633-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
AB Hexakis(trifluoromethyl)benzene (I) was obtained in 70-5% yields by heating hexafluoro-2-butyne (II) with F3Cl (III) or iodine at 260° under pressure. II (11.1 g.), 1.8 g. III, and 0.3 ml. perfluorodimethylcyclohexane in a Pt tube under N heated 15 hrs. at 260° and 1000 atmospheric pressure, the mixture cooled to 0°, filtered, and the solid dried gave 7.89 g. I, m. 209-10°. Replacement of III with iodine gave a 70.5% yield of I, infrared bands at 8.1-8.3, 8.51, 9.51, weaker bands at 7.12, 7.43, 7.61, and 7.73 μ. I was also studied by the x-ray diffraction method. II (25 g.) heated 7 hrs. at 275° and 7 hrs. at 285° in a bomb with pressure drop from 905 lb./sq. in. to 390 lb./sq. in., and the product isolated and sublimed at 2 hrs. 100°/1 mm. gave 3.53 g. I. I (5.5 g.) in 1 l. hot alc. treated with 1/3 of a solution of 35 ml. alc. and 2 ml. H2O during 20 min., the rest I (5.5 g.) added slowly, left overnight at room temperature, the volume reduced to 150 ml., the hot solution decanted from precipitated KF, and cooled gave 4.22 g. Et pentakis(trifluoromethyl)benzoate, m. 89-90° (pentane). Attempts to isolate other hydrolysis products from this reaction were unsuccessful. I was resistant to hydrolysis by H2SO4 or by chlorosulfonic acid-H2SO4.
IT **862-54-4**, Benzoic acid, pentakis(trifluoromethyl)-, ethyl ester (preparation of)
RN 862-54-4 CAPLUS
CN Benzoic acid, pentakis(trifluoromethyl)-, ethyl ester (6CI, 8CI) (CA INDEX NAME)